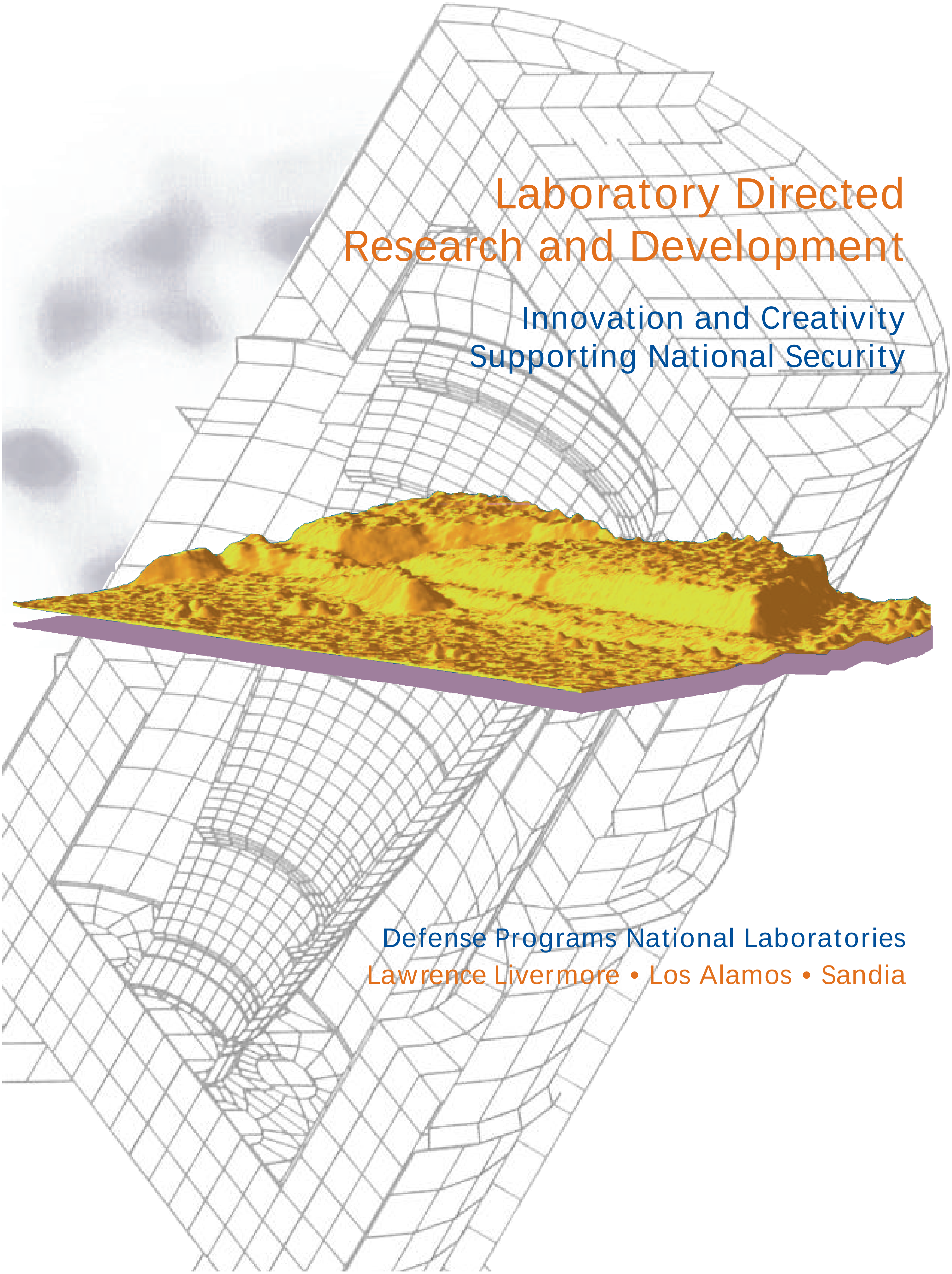
Laboratory Directed Research and Development

Innovation and Creativity Supporting National Security



Defense Programs National Laboratories
Lawrence Livermore • Los Alamos • Sandia

Cover
(foreground to background): Image from a spaceborne synthetic aperture radar used for surveillance and topographic mapping; three-dimensional spatial mesh used to simulate damage to a nuclear weapon and its shipping container when impacted on a rigid wall; image from a gamma-ray imaging spectrometer used to count warheads on emplaced missiles.

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Acknowledgment: Dan Bergbauer, DOE/DP, made valuable contributions to the evolution of this document.

This report presents an overview of the Laboratory Directed Research and Development (LDRD) programs at the three Department of Energy (DOE) nuclear weapons national laboratories: Lawrence Livermore (LLNL), Los Alamos (LANL), and Sandia (SNL). The report focuses on the role of LDRD in supporting the national security mission of DOE by these national laboratories. The report is a product of the Defense Programs LDRD Working Group, which consists of representatives of the three national laboratories, the cognizant DOE operations offices [Albuquerque (AL) and Oakland (OAK)], and DOE Headquarters (Defense Programs).

LDRD Working Group meeting at Lawrence Livermore Laboratory
December 10, 1996

back row: John Vigil, LANL, Dan Bergbauer, DOE/DP, Ed Heighway*, LANL, Nathan Lucas*, DOE/OAK, John Brewer, SNL, *front row:* Lucille Gentry, DOE/AL, Mauri Katz*, Chair, DOE/DP, Rokaya Al-Ayat*, LLNL, Stacey Blaney, LLNL, Chuck Meyers*,SNL, *not present:* Larry Adcock*, DOE/AL

* principal member

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Preface

For over half a century, we have maintained the reliability and safety of the Nation's nuclear weapons stockpile through a strategy of surveillance, nuclear and nonnuclear testing of both stockpiled and new weapons, and an active program of new warhead design and production and replacement of old weapons. With the end of the Cold War and the advent of a Comprehensive Test Ban Treaty, we had to develop a new approach for ensuring the Nation's nuclear deterrent. This approach, Science-Based Stockpile Stewardship (SBSS), requires a more fundamental, in-depth understanding of all the science, materials, and engineering basic to nuclear weapons, as well as the capability to remanufacture or refurbish weapons in the enduring stockpile. Success of SBSS depends upon the Nation's stewards of nuclear weapons, the three nuclear weapons national laboratories: Lawrence Livermore, Los Alamos, and Sandia.

The strategic value of the three nuclear weapons national laboratories lies in their world-class science, technology, and engineering. These capabilities, which constitute a national resource, must stay on the cutting edge because the safety, security, and reliability of the Nation's nuclear weapons depend directly on them. Key to maintaining the vitality of the nuclear weapons laboratories, moreover, is Laboratory Directed Research and Development (LDRD).

The LDRD program provides the laboratory directors with the needed flexibility to invest in longer-term, higher-risk, and potentially higher-payoff research activities that stretch the science and technology capabilities of the laboratories. This report highlights contributions from the LDRD programs at the three nuclear weapons national laboratories in supporting the implementation of SBSS and the overall national security mission.

Victor H. Reis
Assistant Secretary for Defense Programs
Department of Energy

I. Role of Laboratory Directed Research and Development at the Nuclear Weapons National Laboratories

Authorized by Congress to Maintain Laboratory Vitality

In 1990, the Congress of the United States recognized* the importance of laboratory director-initiated research and development (R&D) at the Department of Energy (DOE) national laboratories in the form of a program called Laboratory Directed Research and Development (LDRD). The Congress authorized LDRD expenditures to a maximum of six percent of the funds provided to the laboratories for national security activities. This 6% rate compares to the approximately 2% to 20% typically invested in R&D by industry in the United States. LDRD is mandated to be creative and innovative R&D to ensure the scientific vitality of the laboratories in defense-related scientific disciplines. The three nuclear weapons laboratories, Lawrence Livermore, Los Alamos, and Sandia, make use of the LDRD program primarily to strengthen their science and technology foundations in support of their overall national security mission.

Supports the National Security Mission

The nuclear weapons laboratories have contributed substantially to ending the Cold War by developing the science and technology underpinning the nation's nuclear deterrent capability. Today, the laboratories' main mission is to reduce the global nuclear danger. This they do by being stewards of the nuclear weapons stockpile, by managing nuclear materials, and by seeking ways to reduce and counter nuclear proliferation. These activities are part of DOE's Stockpile Stewardship Management Program. Ensuring that the nuclear weapons stockpile remains safe, secure, and reliable in the absence of nuclear testing is a technical challenge perhaps greater than any the laboratories have faced. Meeting this challenge requires innovative science and technology with the laboratories continuing to advance in areas such as:

- atomic, nuclear, and plasma physics;
- chemistry and materials science, including special nuclear materials (SNM) and other advanced materials under normal and extreme conditions of temperature and pressure;
- radiation (neutron and photon) transport and thermohydrodynamic methods;
- precision and advanced manufacturing;
- sensors, instrumentation, miniaturized electronics, and diagnostic tools;
- lasers and particle accelerators;
- state-of-the-art computers, numerical modeling, simulation techniques, and computer networks; and
- environmental science and bioscience.

LDRD has contributed to each of these areas and is relied upon as an integral and critical component of the scientific research supporting the national security mission. By funding diverse, challenging, and relevant science, the LDRD program is a major vehicle for attracting and retaining the most qualified scientific personnel, as well as for interacting with universities, industry, and other scientific and research institutions.

*Public Law 101-510, 42 U.S.C., known as the FY 1991 National Defense Authorization Act

Focuses on Cutting-Edge R&D for the Future

By any measure, the nuclear weapons laboratories are among the world's great science and technology institutions and are critical to the Nation's science and technology infrastructure. Their capabilities have allowed them to successfully solve the most complex problems, especially those related to national security. Beyond their contributions to nuclear deterrence, the laboratories have made major contributions to conventional defense, nuclear fission power, inertial and magnetic confinement fusion, nuclear propulsion, alternative energy sources, and environmental technology.

The primary focus of LDRD is higher-risk and potentially high-reward R&D for the future—projecting beyond the more specific, near-term, programmatic requirements. By creating and maintaining a solid science and technology base, LDRD allows the laboratories to create new ways of fulfilling their mission and to respond rapidly to evolving and emerging national needs as they arise. Some examples of recent LDRD projects are fundamental studies in aging of nuclear materials, modeling of complex systems, fundamental studies of actinides, high-temperature superconductivity, accelerator production of tritium, advanced dynamic radiographic science, remote sensing science and technology, bioremediation, and quantum information systems.

Produces Exceptional Levels of Scientific and Technological Output

As measured by refereed scientific publications, R&D 100 Awards, and patent applications, the LDRD program produces exceptional levels of scientific and technological output—about five times more than what would be expected on the basis of its percentage of laboratory funding. The data for these metrics, shown for FY 1995, are also representative of previous fiscal years.

LDRD researchers have made, and continue to make, many important contributions in fundamental and applied science relevant to nuclear weapons technology, nuclear materials, defense nuclear waste

Percent Attributable to LDRD (FY 1995)

	Refereed Publications	R&D 100 Awards*	Patent Applications
Los Alamos	53	67	35
Lawrence Livermore	32	40	25
Sandia	12	75	38

*In a world-wide competition, *R&D Magazine* annually selects the 100 most significant products, materials, processes, software, and systems with commercial promise.

disposal, nonproliferation, counterproliferation, and conventional defense through the most innovative science and technology. These in turn have enabled important advances for the core national security programs. Some of these contributions are highlighted in Sec. II, with additional detail and other examples given in the Appendix.

Maintains a High Level of Accountability

The Office of the Assistant Secretary for Defense Programs, together with the Albuquerque and Oakland Operations Offices, hold the three weapons laboratories strictly accountable for management of their LDRD programs through formal requirements and active oversight. The requirements include annual approval of program plans and funding levels, annual program reviews and reports, and annual certification of methods for accumulation of funds. Each laboratory has a formal process for managing its LDRD program that includes calls for proposals, peer and scientific management reviews, and project selection procedures. In addition, representatives from the three laboratories and the DOE oversight offices compose a working group that meets quarterly to share information, encourage collaborations, and address and resolve issues of mutual interest.

Has Added Value as a Separate Program

LDRD has been created as a program separate from the ongoing directly funded programs, which follows best practice in research organizations worldwide. This deliberate separation provides several important benefits. It offers the institutions the opportunity to stand back from the near-term urgencies of current programs to take a strategic look at the health of, and prognosis for, their science and technology and their key resources. It further offers the opportunity for the institutions to execute multidisciplinary, multiprogram research that explores their toughest scientific problems in a multifaceted way. But most importantly, it solicits the most innovative science and technology from the full scientific expertise of the institution, often looking beyond the horizon of the immediate science and technology environment to create genuinely new capability. In this report, there are several examples of LDRD research that were initiated to answer a scientific question and that subsequently found important but unforeseen applications to programs in both the defense and commercial sectors. ■

Laboratory Directed R&D

- strengthens the science and technology foundations of the nuclear weapons laboratories
- helps attract and retain top-level scientific personnel
- allows the laboratories to respond rapidly to emerging national needs
- supports the DOE national security missions as well as civilian applications
- uses peer and scientific management reviews to select projects
- maintains a high level of accountability

II. Highlights of Contributions of Laboratory Directed Research and Development to National Security

The three nuclear weapons laboratories conduct LDRD programs that contribute substantially to their cutting-edge capabilities in nuclear weapons science and technology; nonproliferation, counterproliferation, and arms control; nuclear materials characterization and defense waste disposal; and other national security areas such as materials, detectors, and computational tools for defense applications. In this section, we highlight a few examples of LDRD contributions in these areas; additional details and other examples are presented in the Appendix.

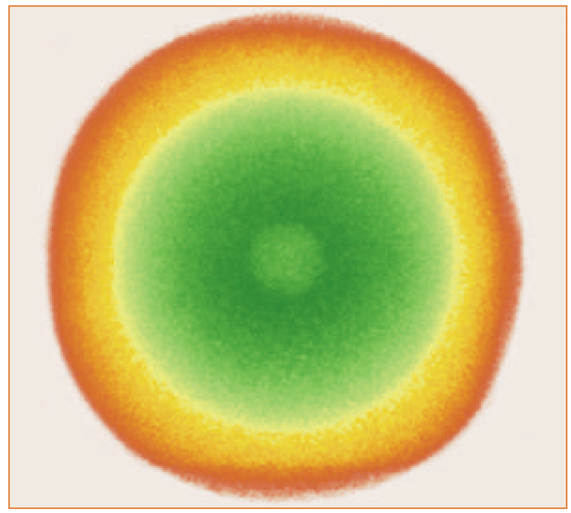
Nuclear Weapons Science and Technology

LDRD researchers are

- developing new and innovative imaging and diagnostic techniques to augment traditional x-ray radiography for stockpile stewardship and surveillance;
- advancing the fundamental understanding of special nuclear materials with recent emphasis on the effects of aging;
- developing environmentally friendly and more efficient approaches to remanufacturing and refurbishing nuclear weapon components in the enduring stockpile;
- developing advanced methods for modeling and simulating nuclear weapons with high fidelity; and
- advancing the state of the art in supercomputing.

New Imaging/Diagnostic Techniques for Stockpile Stewardship and Surveillance

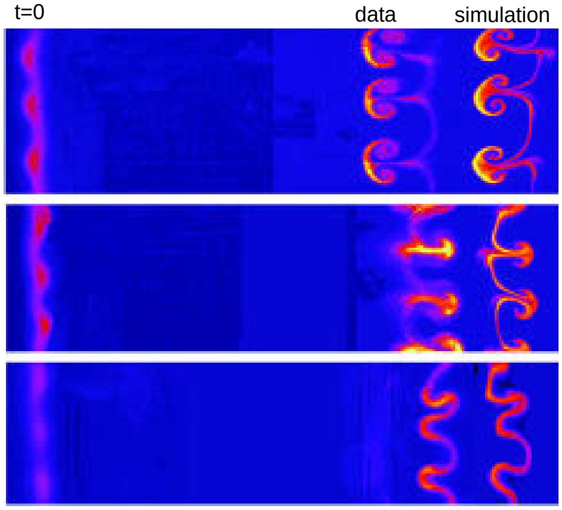
Without nuclear testing, our fundamental understanding of the underlying science of nuclear weapons performance must be improved. LDRD researchers are developing new diagnostic techniques for stockpile certification and for improving the modeling capability of our nuclear weapons codes. Below, we highlight two new diagnostic techniques: proton radiography and laser sheet illumination.



Proof-of-principle proton radiograph of a static test object using high-energy protons.

Proton Radiography. Recently, LDRD researchers identified a promising new approach for making high-resolution radiographs of very rapid events in high-density materials using high-energy protons. Proton radiography complements neutron and x-ray radiography and has the potential for providing tomographic movies of an implosion of a simulated warhead. Its advantages are high spatial resolution, sensitivity to density variations, and the ability to capture the time history of the implosion. LDRD has funded a proof-of-principle test that produced proton radiographs of a dense, **static** object. LDRD scientists are now developing the capability to make **dynamic** radiographs of dense objects under explosive compression.

Laser-Sheet Illumination. The tendency of adjacent but dissimilar liquid layers to interpenetrate and mix together (interface instability) is a problem of central importance to nuclear weapons performance and simulation. In particular, interfacial



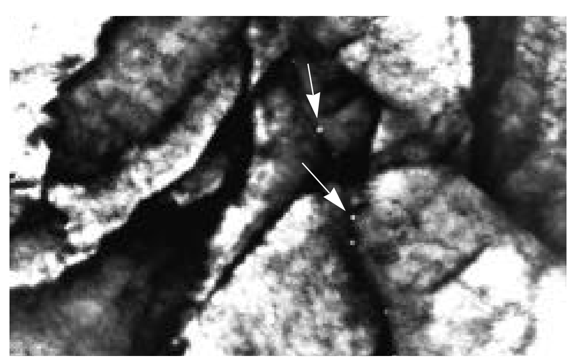
MILSI-measured and computed instability of a thin fluid layer driven by shock compression.

instability of a thin fluid layer driven by shock compression is a fundamental issue in understanding turbulent mixing in nuclear weapons. LDRD researchers are developing a new measurement technique, called multiple imaging of laser-sheet illumination (MILSI), to obtain "snapshots" of the evolving instability. The information obtained with MILSI leads to more accurate simulation models and improved computational results. This technology complements traditional x-ray radiographic methods and enhances the diagnostic capabilities for non-nuclear hydrodynamic tests, as well as improving the ability to predict nuclear weapon performance.

Aging Effects in Nuclear Weapon Components

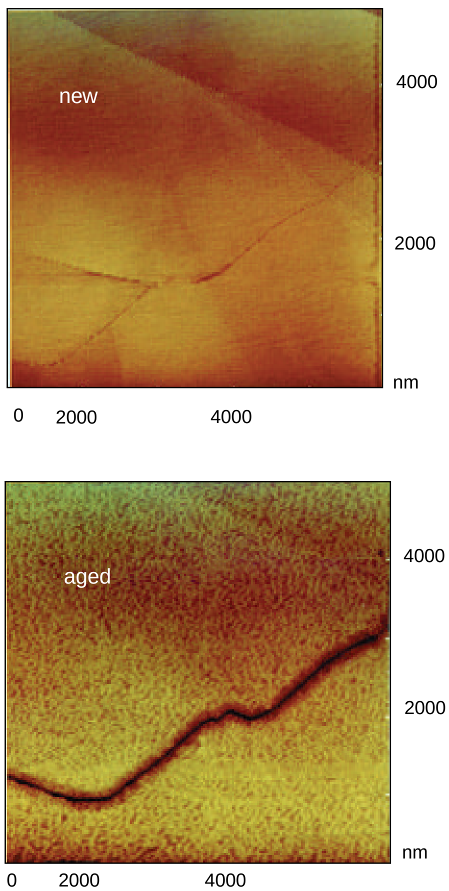
Understanding the effects of aging on nuclear weapon components, particularly plutonium and polymers, is a very important aspect of Science-Based Stockpile Stewardship (SBSS). LDRD researchers are making substantial contributions to this understanding through theoretical, computational, and experimental analyses.

Plutonium Aging. The effect of helium ingrowth (from alpha decay) on the integrity of plutonium as it ages is an important issue in stockpile stewardship and recertification. Of particular interest is the metallurgical condition of the metallic lattice and substructural features such as the accumulation of helium bubbles at grain boundaries. Such defect structures are known to affect swelling and cracking in other materials, and they may negatively influence the mechanical properties of plutonium under high-strain-rate conditions. LDRD researchers are investigating helium bubble formation and distribution in aged plutonium metal using transmission electron microscopy, small-angle neutron scattering, and other advanced techniques. They are also developing the computer simulation tools to evaluate the effect of this and other aging phenomena on properties that are germane to nuclear weapons safety and performance.



Helium bubble formation in plutonium.

Polymer Aging. Degradation of polymers as they age is probably the most important factor in limiting the lifetimes of stockpiled



Materials aging research: grain boundary corrosion in high explosive.

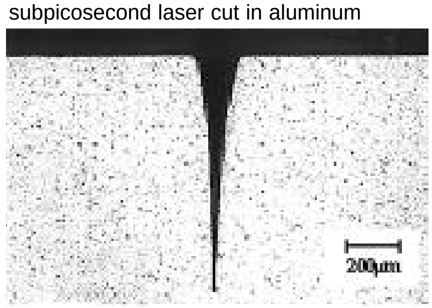
weapons. LDRD researchers are using both experiment and theory to link the large span of scales needed to predict accurately how changes in chemical structure, physical structure, and state of stress impact the mechanical properties of the materials. Although some aspects of each of the size scales (atomic, molecular, mesoscale, microscale, and macroscale) have been studied in the past, LDRD researchers are making one of the first attempts to link this wide range of size scales into a coherent picture that can be used to understand the fundamental behavior of polymeric elastomers. The improved understanding of polymer aging phenomena, such as crack formation and propagation, can be directly applied to predicting the useful lifetimes of nuclear weapon components.

Advanced Manufacturing Processes Relevant to the Weapons Program

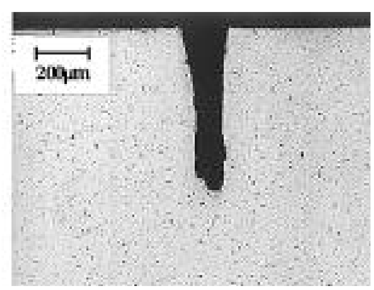
LDRD researchers are making substantial contributions to advanced manufacturing technologies that are directly relevant to the nuclear weapons program. These technologies include high-power lasers to perform delicate and sophisticated machining operations on nuclear weapons components; laser-aided deposition of metals to fabricate component parts to near-final tolerance with no waste generation; and fast-casting technology that bypasses traditional machining operations.

Laser Machining and Stockpile Management. Maintaining the safety, reliability, and effectiveness of the enduring nuclear stockpile will require remanufacturing

subpicosecond laser cut in aluminum



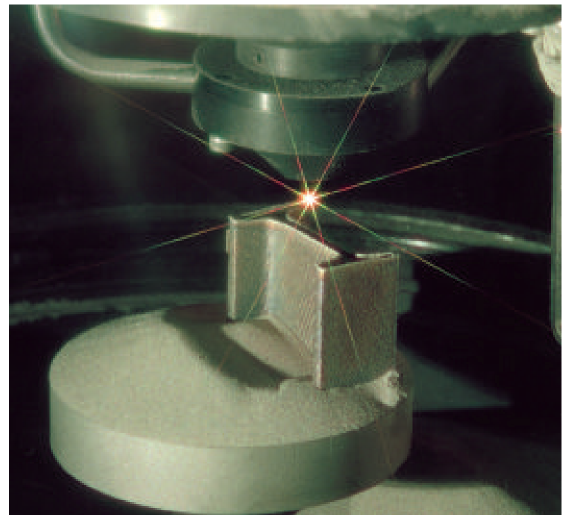
conventional laser cut in alu-



Subpicosecond lasers can cut with no collateral damage, higher precision, and higher efficiency than is achievable with conventional lasers.

and refurbishing of components as the weapons age. LDRD researchers have developed advanced lasers to perform sophisticated and delicate machining activities. The early focus of these LDRD activities developed a theoretical understanding of laser-metal interactions. This knowledge has led to realistic simulation models, which have been validated by comparisons with experiments, and to an in-depth understanding of the appropriate laser parameters for specific machining applications. In particular, LDRD basic research in short-pulse, laser-beam interactions with material provided information, which, when used with the laser-materials machining codes, indicated that very accurate material cutting was feasible. Results from these investigations led to the development of a high-power (petawatt or 10^{15} watts), short-pulsed (less than a picosecond or 10^{-12} s) laser that can cut special nuclear materials with the required fine precision, making it possible to remanufacture and refurbish weapons systems in an environmentally benign and cost-effective manner. Development of the petawatt laser has led to subsequent program funding for classified applications in weapons remanufacture that will save the Nation hundreds of millions of dollars.

Directed-Light Fabrication of Weapon Components. LDRD researchers have developed a new fabrication process called directed-light fabrication (DLF) and are exploring its application to nuclear weapons fabrication (beryllium, uranium, and plutonium components). The DLF process is an automated, rapid, one-step method of making complex metal parts by fusing metal powder in the focal zone of a laser beam. A positioning system, programmed for each part's design, moves a laser beam along the contours of the part as metal powder is fed into the beam spot and fused, one layer at a time. The resulting parts are fully dense, have excellent structural properties, and are shaped to within a few thousandths of an inch of final tolerance without the use of a mold, pattern, or forming die. The system is highly flexible; operators can change to new shapes by downloading a new computer file into the positioning system. The high-energy density of the laser permits fusing of any metals including refractory metals that are hard to form with conventional techniques. The process is ideal for low-volume production of precision parts for both defense and civilian applications. This LDRD-developed process won an R&D 100 award in 1994.



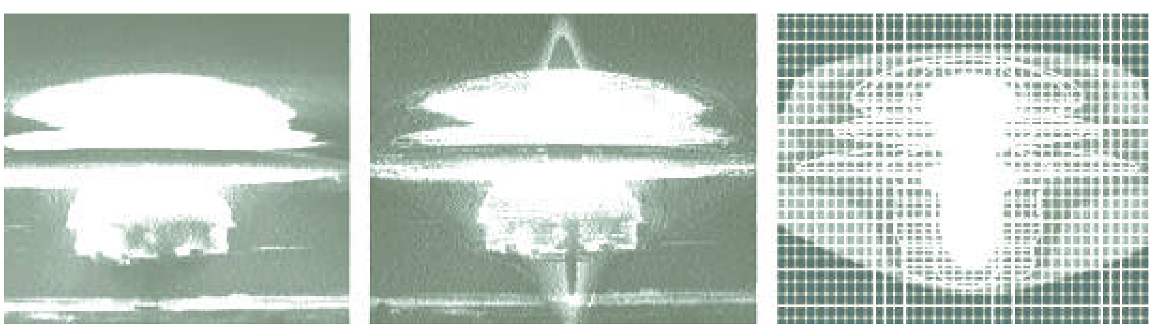
Directed-light fabrication of complex metal parts.

Casting Technologies. LDRD researchers have provided enabling technology for a process, called FastCast, that allows very rapid production of stockpile-quality fireset housings for nuclear weapons. FastCast integrates computational simulation, rapid prototyping, and casting technologies into an architecture that enables the designer to go from "art to part," bypassing traditional machining operations. The FastCast technology has made possible the delivery of fireset housings within ten working days of receipt of the electronic design (about 20 times faster than previously possible).

In another related LDRD effort, scientists are developing improved casting processes using ambient-temperature molds and numerical tools to predict phase transformation, thermal behavior, residual stresses, and distortion during plutonium casting. If proven practical, the ambient-temperature mold concept will simplify casting-furnace design and reduce the heat-treating time necessary to produce the required homogeneity in the plutonium part. This LDRD effort is also developing computer simulation programs to predict distortion, residual stress, and thermal management in cast plutonium parts. Advances in these areas will benefit both the Advanced Design and Production Technology (ADaPT) and Accelerated Strategic Computing Initiative (ASCI) programs of the DOE.

Advanced Computational Capability and Nuclear Weapons Simulation

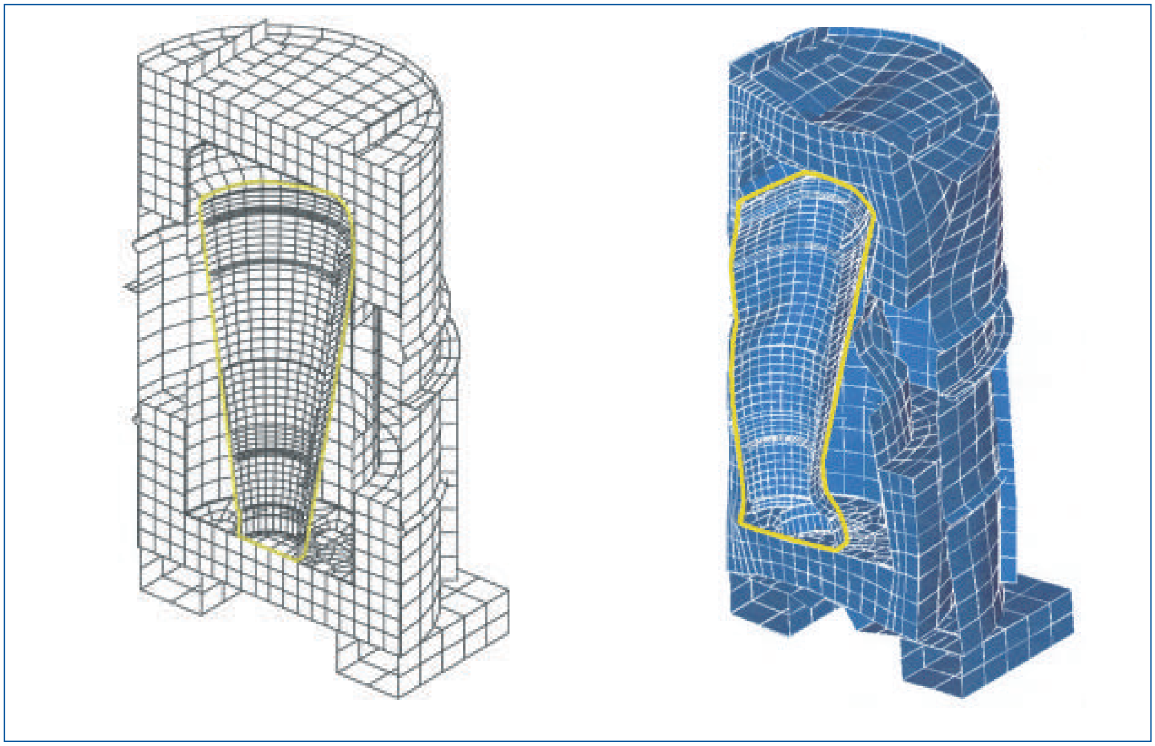
The ability to predict with confidence the performance of nuclear weapons based on computer simulations and nonnuclear experiments is key to maintaining a safe, secure, and reliable stockpile in the absence of nuclear testing. Computer simulations of the complex phenomena that occur in a nuclear explosion continue to tax available state-of-the-art computational capabilities and simulation techniques. LDRD researchers are developing advanced methods and tools to model radiation, material, and heat flows in nuclear devices. On a broader front, they are exploring advanced computing technologies and advancing the state-of-the-art computational capabilities at the three nuclear weapons laboratories.



Evaluation of nuclear weapon effects has shifted from nuclear tests to nonnuclear experiments and computer simulations (shown are atmospheric effects).

Nuclear Weapons Simulation Methods. LDRD researchers developed the discrete ordinates (Sn) method for radiation transport, the particle-in-cell method for hydrodynamics, and other computational tools that are now used widely in both military and civilian applications. Today, LDRD researchers are providing the technology to implement these tools on the new generation of massively parallel supercomputers. They are also extending the capability of these tools through new developments such as a complex geometric representation common to both Monte Carlo (MC) and Sn codes; an automatic, three-dimensional MC variance-reduction algorithm; a massively parallel, high-order-accurate, deterministic transport method capable of modeling complex, three-dimensional geometries; innovative algorithms involving volume/interface tracking, advection, and interfacial flow for improved simulation fidelity and efficiency; and new adaptive mesh refinement techniques such as the one described below.

Engineers design and simulate the performance of new products, whether automobiles or nuclear weapons, by first creating a spatial-mesh model of the object. This mesh-generation task has traditionally been a highly challenging and time-consuming portion of the overall analysis. Approaches to

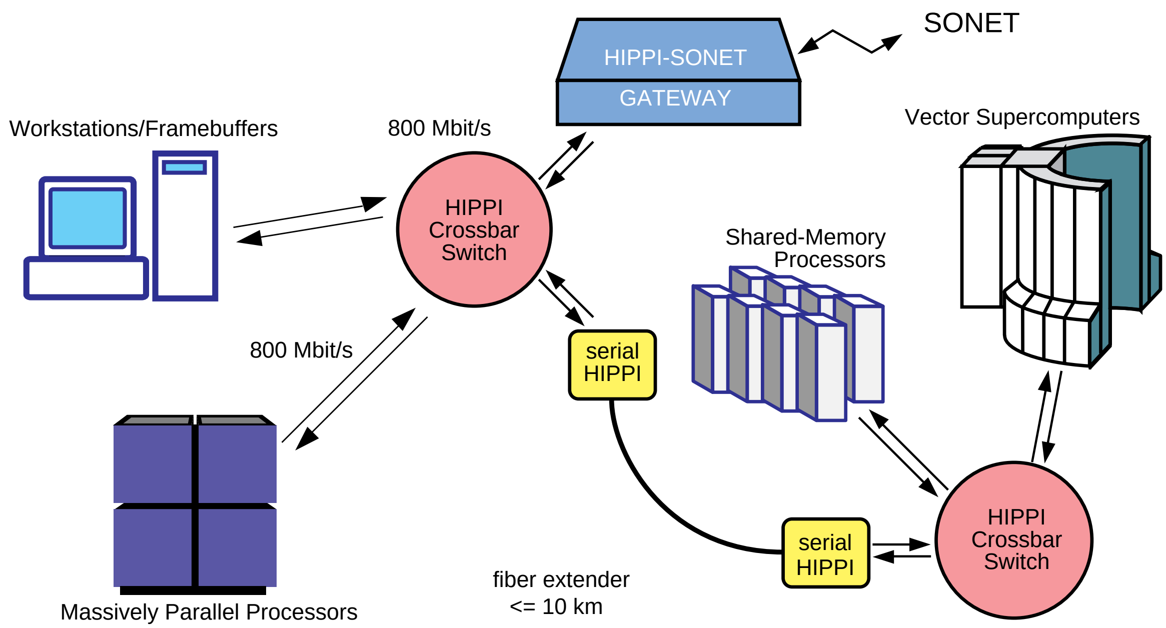


Sample spatial mesh used to simulate damage to a nuclear warhead and its shipping container in an impact with a rigid wall.

solving this problem have been investigated by LDRD researchers, and one outcome is a new patented algorithm called "paving," which fills an arbitrary, three-dimensional surface with quadrilateral elements. This all-quadrilateral mesh can be made both very efficient and accurate, and for complicated cases, the algorithm can produce a mesh three to ten times faster than current manual methods. Paving can also be used to modify and improve a mesh during analysis, a process called adaptivity, which can take the guesswork and error out of constructing a finite-element mesh.

Data-Transfer Network and Multimedia Technology. Computer simulations of nuclear weapons require not only the most powerful computers available, but also the ability to transfer huge amounts of computational data and the capability to display this data in forms that can be more easily digested and analyzed. LDRD researchers have advanced the state of the art in fast, data-transfer network technology by inventing the high-performance parallel interface (HIPPI), which supports local networks at data-transfer rates of 800 million bits per second (equivalent to one-hundred, 250-page books per second). HIPPI has been adopted as a standard by the American National Standards Institute, and it is currently the high-speed interface of choice for supercomputers. Building on this LDRD work, a synchronous optical network (SONET) gateway has been developed that can link supercomputers at HIPPI speeds over very large distances. This invention received an R&D 100 Award in 1995.

LDRD researchers have also contributed to the understanding of traffic-management issues in high-speed, asynchronous-transfer-mode (ATM) networks by developing an MC simulator that models the various components in such a network. ATM technology is the basis upon which the Defense Programs' high-performance ASCI network is being designed.



HIPPI-SONET Gateway enables distributed supercomputing to address complex problems.

Nonproliferation, Counterproliferation, and Arms Control

LDRD researchers are advancing the science and technology required to verify and monitor arms control treaties and to help detect the clandestine production of weapons of mass destruction such as nuclear, chemical, or biological weapons. Highlighted in this section are

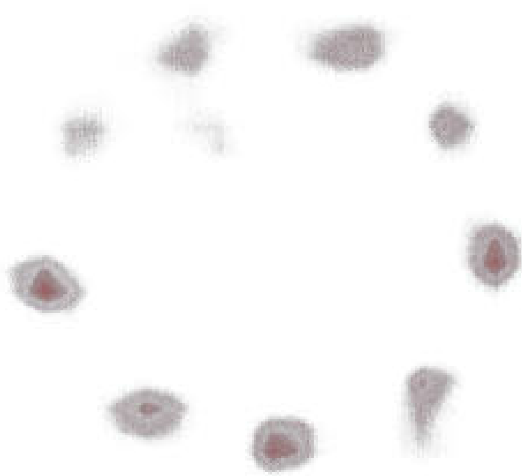
- a gamma-ray imaging detector that has found application in the arms inspections called for by the Strategic Arms Reduction Treaty,
- techniques for distinguishing signals from a clandestine nuclear explosion from signals generated by natural phenomena such as lightning,
- a suitcase-sized gas chromatograph/ mass spectrometer for on-site identification of ultrasmall traces of certain compounds, and
- a computer-based tool for modeling the global management, control, and flow of weapons-grade nuclear materials.

Advanced Gamma-Ray Detectors

In the early 1990s, LDRD funded research on new types of gamma-ray detectors, imaging gamma-ray cameras, and the computer analysis of signals from networks of detectors. Much of this work was initially motivated by fundamental astrophysical investigations, but it has subsequently found its most important applications in counterproliferation and treaty verification. One particularly important development is a gamma-ray imaging spectrometer (GRIS), which can be used to count the number of warheads on board a missile without requiring either close access to the missile or its disassembly. Related applications that take advantage of GRIS's ability to "see" behind shielding occur in the characterization and safeguarding of nuclear weapons and in nuclear waste disposal.

Configuration for GRIS imaging of a Peacekeeper missile.

GRIS image from an emplaced Peacekeeper missile carrying ten warheads.

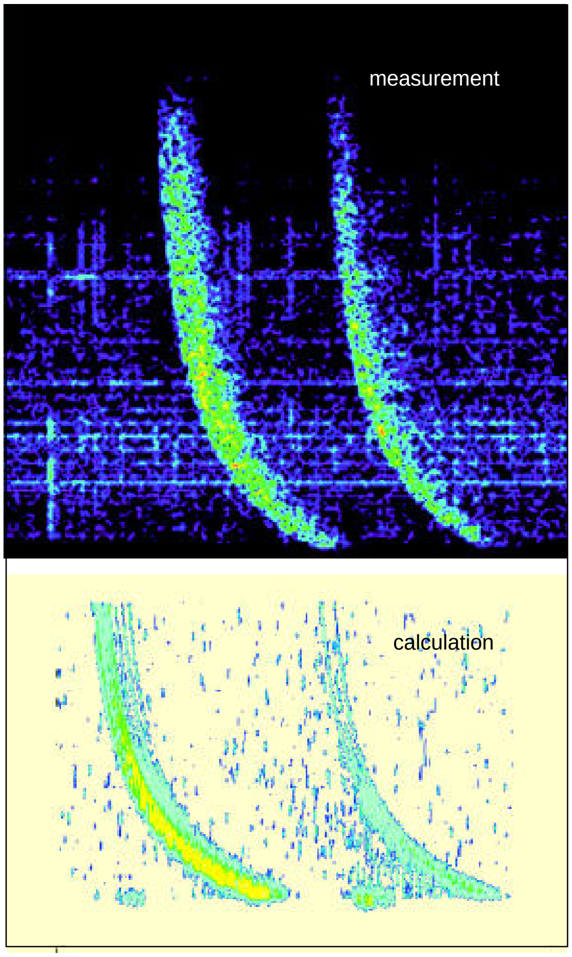


Another LDRD-funded development, nonimaging detectors, is also finding application in counterproliferation activities. These detectors can track the movement of a "clandestine" nuclear weapon by using a sophisticated tracking algorithm to identify the weapon's signal in a high-background environment. Eventually, this approach could be used in civilian areas such as seaports, airports, and other high-risk but constricted areas.

Detection of Clandestine Nuclear Explosions

Earth-orbiting satellites have detected transionospheric pulse pairs that are similar to signatures generated by a nuclear explosion. LDRD scientists have now shown that these signals can be explained by a runaway electron mechanism near thunderstorms that causes upward-propagating discharges called "sprites." The new theory agrees with measurements of radio-frequency "chirp" pairs, as well as with optical and x-ray emissions associated with this phenomenon. This understanding will allow scientists to more accurately identify signals from clandestine nuclear explosions.

LDRD researchers are also developing a method to detect clandestine nuclear explosions in the upper atmosphere based on the detection of low-frequency (subaudible) sound waves, which can travel and be detected at great distances. These subaudible sound waves are rare in nature, but are generated in aboveground nuclear explosions and can be detected worldwide with the properly designed monitoring system. The researchers have used subaudible sound waves generated by space shuttle launches to test, refine, and determine how to deploy detection equipment and how to optimize ways to analyze the data.



Theory of 'sprites' fits measured rf 'chirp' pairs (shown) as well as optical and gamma-ray pulses.

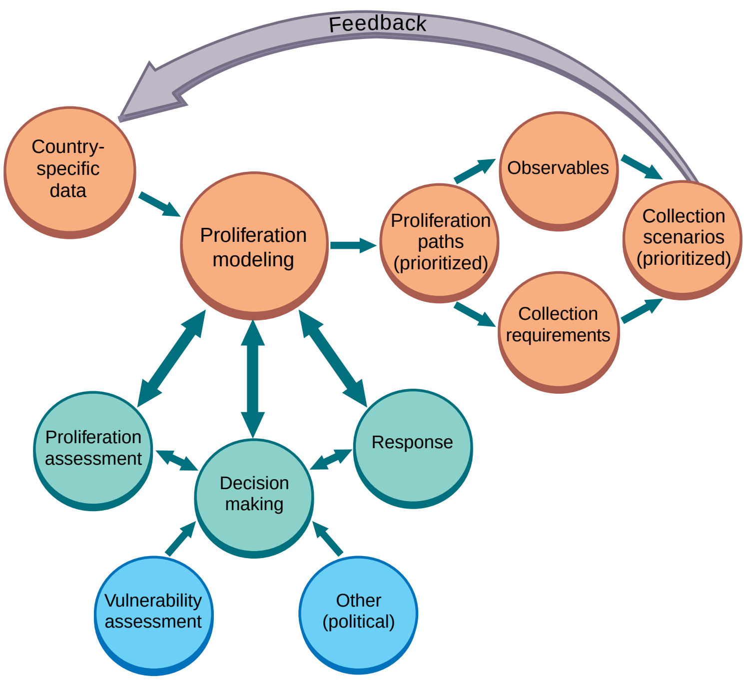
System for Detecting Trace Materials Indicative of Proliferation

LDRD has funded research to determine how best to measure trace materials for nonproliferation, counterproliferation, and other purposes. Using sophisticated analytical equipment, researchers in organic, inorganic, and biochemistry invented and demonstrated new ways to determine the composition and, often, the sources of the most minute samples of unusual materials. One such example is development of a portable, suitcase-sized gas chromatograph/mass spectrometer (GC/MS) for on-site identification of ultrasmall (microgram or less) quantities of certain compounds in complex mixtures. The system weighs 20 kilograms, including an accompanying laptop computer, can be carried onboard an airplane, and can be placed into the overhead compartment. Meanwhile, its accompanying generator and off-line vacuum-reconditioning pumping unit travel in the baggage compartment. This LDRD-developed system is finding application in nonproliferation activities.

Suitcase GC/MS system.

Global Nuclear Material Flow Model

The global proliferation of weapons-grade plutonium and highly enriched uranium has become one of the foremost threats to global security. LDRD researchers are characterizing and modeling, from a global perspective, the management, control, and



LDRD researchers are developing tools to help understand the management, control, and flow of weapons-grade nuclear material.

flow of weapons-grade nuclear materials. The objective of this research is to provide a computer-based tool capable of capturing and enumerating data concerning the global inventory of nuclear weapons materials; to provide a global view of the management and control of nuclear materials; to undertake macrosystem simulations of safeguards accounting surety and safeguards resource estimation; and to visually represent the nuclear materials information, including both intercountry and intracountry flows. The researchers have developed a prototype of the fundamental, computer-based framework necessary to undertake these studies. It is expected that this tool will help answer questions concerning the degree of certainty associated with estimating material quantities based on inventory information, safeguards-accounting information, and material transit. It should also provide the framework, initial data, and information necessary for conducting optimization studies to estimate safeguards resource requirements based on the existing safeguards resources, management and control requirements, and changing assurance needs.

Nuclear Materials and Defense Waste Disposal

LDRD-funded activities at the nuclear weapons laboratories have contributed significantly to science and technology advances in nuclear materials and defense waste disposal. In this section, we highlight LDRD contributions to

- the measurement of the melting curve of plutonium,
- advanced methods for processing and recovering plutonium,
- the recovery of actinides and toxic metals from a variety of process streams, and

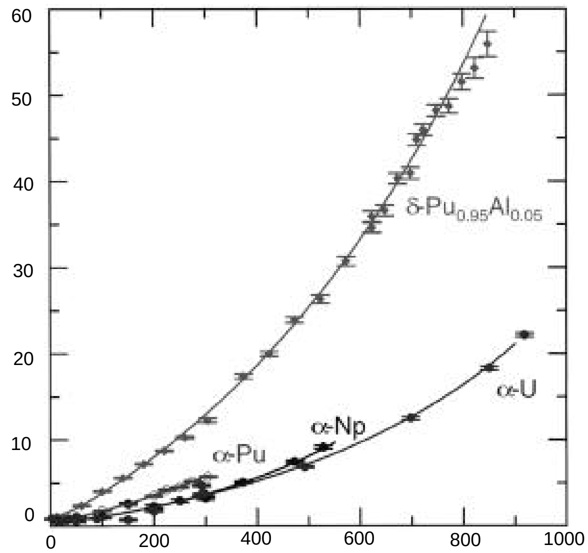
- the development of sensors for monitoring special nuclear materials (SNM).

Plutonium Equation of State

The diamond anvil cell (DAC), invented by LDRD researchers in the 1980s, is a versatile experimental tool for studying the properties of materials at very high pressures. The DAC apparatus is well suited for investigating plutonium and other toxic metals because the samples required are very small (milligrams) and are easily contained. More recently, LDRD researchers developed a laser-heated DAC that allows high-temperature, high-pressure measurements in regimes that previously could only be reached during chemical or nuclear-explosion-driven experiments. The researchers have used the laser-heated DAC to extend the melting curve of plutonium, which has helped solve a long-standing problem in accurately modeling implosion devices. Precise measurements of the melting curve have enabled more accurate simulation of the distribution of solids and liquids in an imploding device, thereby leading to improved understanding of the implosion process and better prediction of device performance.

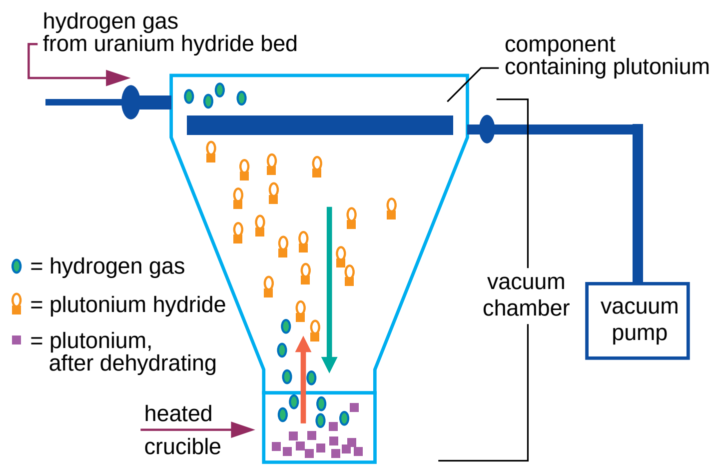
Plutonium Recovery

LDRD researchers are performing a series of laboratory-scale experiments to obtain data for enhancing the operational and safety characteristics of a new process for recovering metallic plutonium from nuclear weapons. The hydride-dehydride recycle process, which won a 1995 R&D 100 Award, eliminates the environmental hazards associated with other plutonium



Debye-Waller factors for plutonium alloys from neutron scattering.

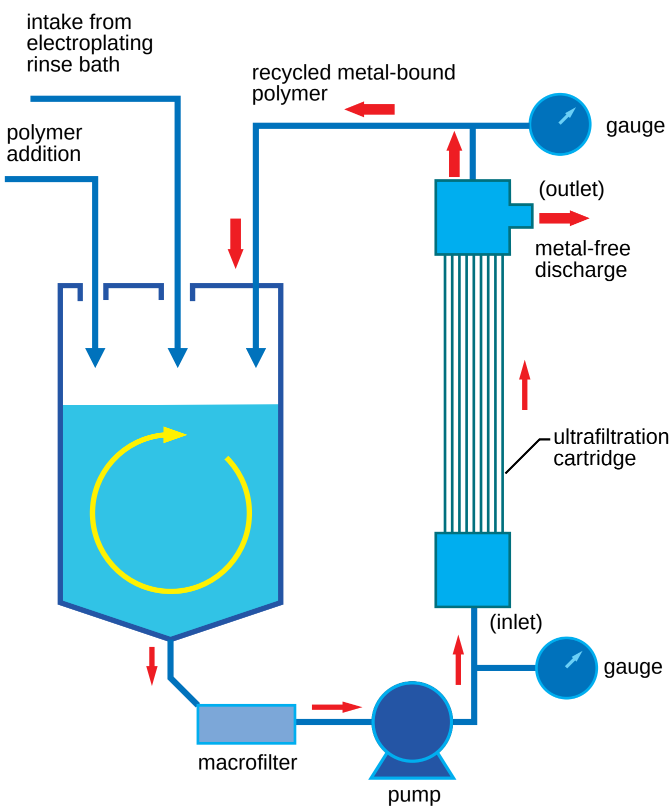
recovery methods. It takes advantage of plutonium's strong affinity for hydrogen gas, a reaction that forms plutonium hydride. The reaction takes place in a vacuum chamber inside a glove box. The lower part of the chamber includes a heated crucible, and the upper part (cold zone)



Hydride/dehydride process for plutonium recycle.

contains the weapon component. A small amount of hydrogen gas is introduced into the cold zone, where it reacts with the plutonium to form plutonium hydride powder. The powder falls into the hot crucible where the hydrogen is released (the dehydriding reaction). The hydrogen then recycles until all the plutonium has been extracted from the weapon component. When the process is complete, the plutonium powder is melted and incorporated into a storage-ready ingot. This LDRD work helps provide core technology for the Advanced Recovery and Integrated Extraction System (ARIES).

In a related LDRD development, plutonium metal is converted to plutonium hydride, which is then chlorinated to form plutonium chloride and volatile chloride impurities. This technology could be used to reprocess plutonium from older nuclear weapons for use in recycled weapons, or it could provide weapons plutonium as purified feed material to be burned in nuclear power reactors as part of nonproliferation. This LDRD effort has resulted in a successful feasibility demonstration that has strengthened the technology base for plutonium processing. This new technology is being considered by the DOE Fissile Materials Disposition Program for removing impurities from plutonium contained in excess pits.



Polymer filtration system for metal-ion recovery.

Polymers for Actinide and Toxic Metal Recovery

The high cost associated with the long-term storage of radioactive and toxic wastes mandates separating these components in a process waste stream before the waste is packaged and stored. LDRD researchers have developed and evaluated water-soluble chelating polymers for recovering actinide and toxic metals from a variety of process streams, as well as polymer filtration for recovering precious metals from industrial process streams. A portable, polymer filtration system based on this technology and used to recover zinc and nickel ions from electroplating rinse waters won an R&D 100 Award in 1995. LDRD researchers are now investigating membrane-based separation technologies for the removal of plutonium and americium from nuclear-materials-processing waste water; fission-product separations using cobalt dicarbolide for solvent extraction; hollow-fiber membrane modules for separating gases and nuclear materials; and selective waste remediation using *in situ* photocatalytic reactors.

Portable Gamma- and X-Ray Detector

LDRD researchers have developed a new, field-portable, x-ray fluorescence (XRF) analyzer, based on large-area mercuric iodide (HgI_2) radiation sensors, for on-site analysis of solid and liquid effluents. The unit consists of a hand-held probe and an XRF analyzer module, which contains a computer, software, and display. The instrument is lightweight, easy to operate, and battery powered; it requires no maintenance for months and is capable of remote, unattended data collection. The XRF instrument also operates as a direct gamma-ray spectrometer, and it has been used to perform nondestructive assays of radioactive gamma-emitting materials such as uranium and plutonium. The high-resolution capability of the HgI_2 sensors allows the instrument to identify radioactive materials by their unique radiological signatures, and it has been used to characterize a wide variety of nuclear materials. The sensors are radiation tolerant, with a damage threshold two to three orders of magnitude higher than cryogenically cooled silicon or germanium detectors; this allows their use in monitoring high-level radioactive waste or in long-term monitoring of weapon pits. Beyond the capability for monitoring stored SNM, the gamma-ray spectrometer can be used to detect nuclear smuggling, to aid in SNM search scenarios, or to perform *in situ* monitoring of airborne radioactive particulates that have been collected on filters.

Other National Security Research Areas

LDRD contributions to other national security areas include research and development of materials, detectors, and computational tools for conventional military applications, as well as sensors for environmental monitoring. In this section, we highlight LDRD contributions to high explosives, ultrasound spectroscopy for nondestructive testing of military components, synthetic aperture radar and advanced target recognition technology, and sensors for monitoring organic compounds.

High-Explosives Research and Development

LDRD-funded researchers have developed numerical models that are routinely used to predict the performance and response of high explosives (HE), especially insensitive HE, which has contributed greatly to the safety of nuclear weapons. This work has led to the development of new shape-charge technology for conventional defense. In addition, LDRD researchers have developed molten-salt technology that is being applied by the military to the safe

and environmentally benign disposal of high
explosives.

Ultrasound Identification of Failure in Military Hardware

Portable field instrument used to rapidly and noninvasively examine and identify the contents of sealed containers.

Resonant ultrasound spectroscopy (RUS) was originally used as a research diagnostic in an LDRD-funded project to measure the properties of high-temperature superconducting crystals. It was quickly determined that RUS could be used for the nondestructive testing of crystals for imperfections in the crystal structure. The technique was further applied to monitor for cracks and other flaws in commercial and military hardware. RUS is now being used for the nondestructive testing of military components (aircraft landing assemblies, turbine disks, helicopter rotor parts, and ball bearings) and for identifying the contents of chemical munitions. Exploratory work is in progress to use RUS to study the effects of aging on hemispherically shaped explosive charges as part of our stockpile stewardship responsibilities

The identification and development of RUS is an excellent example of how LDRD research that was initiated to answer a scientific question can find important applications in both the military and commercial sectors. Applications of RUS built on the foundations provided by the LDRD research have earned RUS several patents and two R&D 100 Awards.

Synthetic Aperture Radar and Automated Target Recognition Technology

LDRD researchers have advanced synthetic aperture radar (SAR) technology by exploring applications of SAR to space;

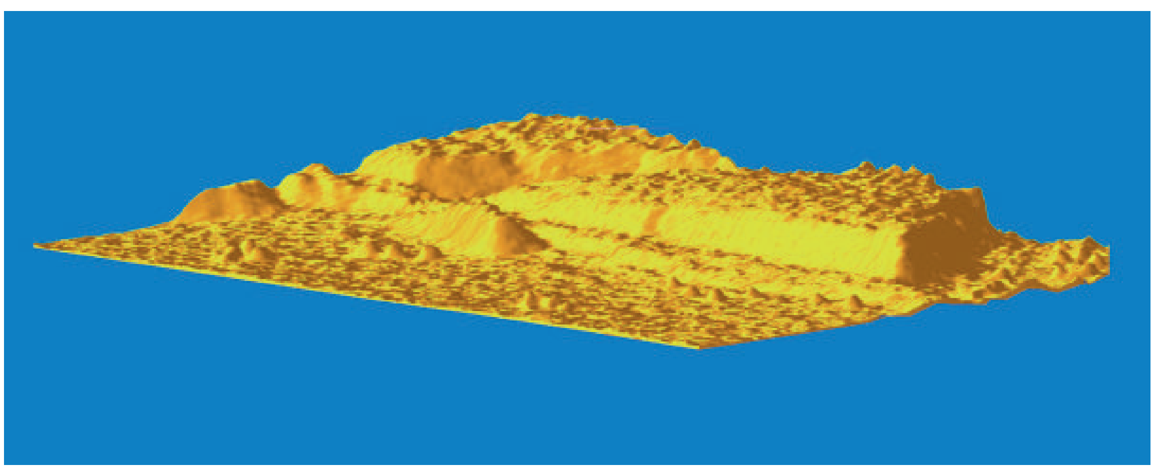
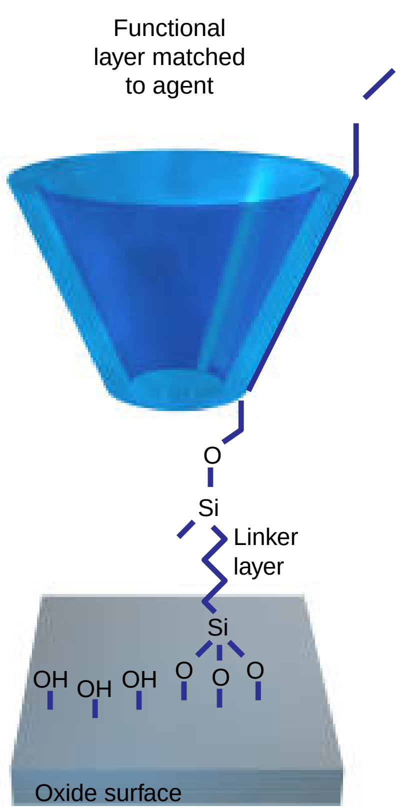


Image from a spaceborne SAR used for real-time surveillance, targeting, and topographic mapping.

developing a unique, three-dimensional interferometric SAR; and extracting target coordinates and features from SAR imagery. As battlefield SAR systems on tactical aircraft become more common, the amount of SAR imagery that must be handled and analyzed will increase dramatically. Handling the increased amount of SAR imagery and the timely identification of time-critical targets, such as mobile SCUD missile launchers, will require automated target-recognition (ATR) systems that can quickly scan the imagery and point out areas of interest for image analysis by humans. LDRD researchers are applying multiple-source data fusion, feature extraction, and neural-net exploration to investigate solutions to the ATR problem.



SAW-based chemical microsensor showing its three-layer (surface, linker, and functional layer) structure.

Sensors for Environmental Monitoring

The LDRD programs at the nuclear weapons laboratories have funded fundamental and applied research on sensors for environmental monitoring of defense wastes and for detecting environmental indicators of weapons production. Using molecular self-assembly techniques, LDRD researchers have developed a compact and robust surface-acoustic-wave (SAW)-based chemical microsensor for remote, real-time reversible sensing of volatile organic compounds. Self-assembly techniques allow toxin-sensing molecules to organize (or self-assemble) so that one end of the molecule bonds directly to a sensing detector (a transducer) and the other end extends as a “bucket” tailored to temporarily trap specific chemicals. Changing the size and polarity of the bucket allows the microsensors to be custom-tailored so that they track specific organic toxins. The organic sensing layer (or bucket) is designed and constructed using molecular-engineered cyclodextrin derivatives, which provide a cone-shaped molecular structure that can readily trap specific organic toxins. Because the cyclodextrin buckets bind the contaminants weakly, the microsensor is reversible and can be used to monitor continuously changing concentrations of the contaminant over

III. Conclusions

an extended period of time. This LDRD-developed technology received an R&D 100 Award in 1995. ■

National Security Relies Strongly on LDRD

The LDRD programs at the nuclear weapons laboratories help ensure the world-class science and technology base needed to address the national goals of enhancing national security and reducing the global nuclear danger.

LDRD solicits the most innovative science and technology from the full scientific expertise available at the weapons laboratories, thereby creating a vital source of new capability. Thus, LDRD contributes significantly to the scientific basis and innovation required for science-based stockpile stewardship, stockpile and nuclear materials management, nonproliferation and counterproliferation, and environmental stewardship, as well as for the civilian missions of DOE.

Because science and technology are expected to continue to play a vital role in the Nation's security, LDRD must remain at the cutting edge to maintain the vitality of the three nuclear weapons laboratories.

LDRD is Essential to Laboratory Capability

With efforts to balance the national budget becoming more intense, and as programmatic funds for supporting research become more scarce, LDRD is being relied upon more and more for the longer-term, higher-risk, potentially higher-return R&D.

As seen from the examples in this report, LDRD delivers cutting-edge science and technology and provides important links to the science and technology communities in government, industry, and academia. This in turn allows LDRD to leverage additional scientific resources and to help attract and retain top scientific talent.

LDRD is Managed in Partnership with DOE

Because of its uniqueness and critical importance to the three nuclear weapons laboratories, LDRD is a prized resource that is managed in close collaboration between the laboratories and DOE. The Department provides policy consistency among the three laboratories. The laboratories have well-defined processes in place for proposal submittal, peer and/or scientific management reviews, and project selection. The laboratories constantly seek ways to leverage their six percent funding allocations to be more productive and responsive to the R&D needs of their programs, particularly to their national security programs.

Both laboratory and DOE management strongly support the vital role LDRD has come to play in accomplishing the national security mission. LDRD has become an integral and essential part of the nuclear weapons national laboratories.■

Appendix

Examples of Contributions of Laboratory Directed Research and Development to the National Security Mission

This appendix contains examples of contributions of LDRD in the areas of nuclear weapons science and technology; nonproliferation, counterproliferation and arms control; nuclear materials and defense waste disposal; and other national security areas. For completeness, the examples highlighted in the body of the report are repeated here, in many cases with additional details.

Additional examples are included to provide the reader with a more complete picture of the range of LDRD activities supporting national security at the three nuclear weapons laboratories. These examples, however, are by no means a comprehensive set of such LDRD activities at the laboratories.

Appendix Contents

Nuclear Weapons Science and Technology

The Laboratory Directed Research and Development (LDRD) programs at the three nuclear weapons laboratories are major contributors to both basic and applied research in a wide variety of scientific disciplines that support nuclear weapons technologies.

Innovative Imaging/Diagnostic Techniques for Stockpile Stewardship and Surveillance

Increased reliance on nonnuclear experiments for stockpile certification, supported by improved computational modeling capability, increases the need for advanced hydrodynamic radiographic capabilities that supplement and complement traditional x-ray radiography. In addition to the two innovative diagnostic techniques described immediately below, LDRD researchers are developing advanced neutron-scattering techniques for application to nuclear stockpile stewardship and surveillance (described in a subsequent section).

Proton Radiography. Recently, LDRD researchers identified a promising new approach that uses protons as the radiographic probe. This approach offers several important advantages over traditional x-ray radiography for investigating explosively driven compression of heavy-metal systems. Some of these advantages are high spatial resolution, sensitivity to density variations, and the ability to capture the time history of the implosion. These capabilities are necessary to address stockpile certification issues definitively without recourse to nuclear testing. LDRD researchers have performed a successful proof-of-principle test of a static test object using 188-MeV protons and are completing a similar experiment using gigaelectronvolt proton beams. To demonstrate proton radiography's true potential for providing tomographic movies of an implosion of a simulated warhead, LDRD researchers are developing and implementing a test capability for dynamic proton radiography.

Laser-Sheet Illumination. The tendency of adjacent but dissimilar liquid layers to interpenetrate and mix together (interface instability) is a problem of central importance to the nuclear weapons and inertial confinement fusion communities. The instability of a thin layer is especially relevant and not well understood. Recent experimental observations of bifurcating flow that is sensitive to initial conditions sparked interest in developing a better understanding of shock-accelerated layers. LDRD researchers are using novel experiments, theory, and numerical simulation to study and understand interfacial instability in interfaces of liquid layers that are shock-accelerated by high explosives. The researchers are detecting these flow patterns by applying a new optical imaging technique (multiple imaging of laser-sheet illumination) to illuminate a two-dimensional slice of a three-dimensional flow field. This technology complements traditional x-ray radiographic methods and enhances the diagnostic capabilities for nonnuclear hydrodynamic tests.

Aging Effects in Nuclear Weapons Components

Understanding the effects of aging on nuclear weapons components, particularly plutonium and polymers, is a very important aspect of science-based stockpile stewardship. LDRD researchers are making significant contributions to this understanding through development of sensors and instrumentation techniques for enhanced surveillance, as well as through theoretical, computational, and experimental analyses of materials in radioactive environments.

Enhanced Surveillance Supporting Research. The understanding of the behavior of materials used in nuclear weapons during long-term storage is a major challenge. LDRD has invested in special sensors and instrumentation techniques to analyze the slow changes in these special materials. This research falls into three major categories: computational analyses of materials exposed to radiation and other harsh environments; instrumentation for atomic-level structural changes; and special sensors for environmental microchanges.

The computational analyses, which are centered on structural changes that occur as special nuclear materials age and slowly decay, are designed to predict the times for refurbishment and change-out of existing parts with new or remanufactured parts.

Instrumentation is represented by the new class of atomic-force and tunneling microscopes, which researchers are using to measure atomic-scale rates of corrosion and materials deterioration. In addition, these instruments have been used to measure the physical properties of organic materials when new, as they slowly decompose, and when they are remanufactured. These measurements allow comparison of computational models of atomic-scale (nanoscale) structures to actual measured systems. Using these techniques, the researchers have been able to measure corrosion rates that are a million times slower than presently observed and calculated. In addition, grain structures can be measured for new and replacement parts.

The final class of surveillance technologies consists of *in situ* sensors that are placed in nuclear weapons and that report on environmental conditions. Examples include sensors that detect the outgassing of hydrogen and organic binder materials within a sealed weapon. Several of the new sensors are read out with fiber-optic techniques, thus preserving the electrical isolation of the systems while allowing continuous, long-term surveillance.

Plutonium Aging. The effect of helium ingrowth (from alpha decay) on the integrity of plutonium as it ages in the stockpile has been identified as an important issue in stockpile stewardship and recertification. Of particular interest is the metallurgical condition of the metallic lattice and substructural features such as the accumulation of helium bubbles at the grain boundaries. These helium bubbles can approach 100 angstroms in size; such defect structures are known to affect swelling and cracking in other materials. Therefore, the helium bubbles may negatively influence the mechanical properties of plutonium (e.g., spall strength) under high-strain-rate conditions experienced with explosive compression. LDRD is currently funding integrated theoretical and experimental investigations aimed at understanding and predicting the formation, growth, and diffusion of helium bubbles and their size distribution in the plutonium metal lattice. In addition to providing a sound understanding of the physics of helium ingrowth in plutonium, LDRD researchers are investigating how this ingrown helium responds to various temporal and environmental conditions, as well as the concomitant effects on plutonium properties.

Polymer Aging. Polymer aging has been identified as the most important materials issue facing extended lifetimes of stockpiled weapons. LDRD researchers have undertaken the challenging task of linking (using both experiment and theory) the large span of size scales (10^{-10} to 10^{-4} meters) inherent in any study of elastomers to accurately predict how changes in chemical structure, physical structure, and state of stress impact the mechanical properties of the system. While some aspects of each of these levels (atomic, molecular, mesoscale, microscale, and macroscale) have been studied in the past, this LDRD work is one of the first attempts to link this wide range of size scales into a coherent picture that can be used to understand the fundamental behavior of polymeric elastomers. The improved experimental and models-based understanding of the science of polymer aging can be directly applied to predicting the lifetimes of weapons components.

Advanced Manufacturing Processes Relevant to the Weapons Program

LDRD has made important contributions to advanced manufacturing technologies relevant to the nuclear weapons program. These technologies include the following:

- laser machining techniques;
- laser-aided deposition of metals to form component parts to near-final tolerance;
- fast casting technology that bypasses traditional machining operations;
- extreme ultraviolet lithography with unprecedented resolution;
- robotics for advanced manufacturing and dismantlement; and
- other manufacturing technologies for special nuclear materials.

Laser Machining and Stockpile Management. Maintaining the safety, reliability, and effectiveness of the nuclear stockpile will require remanufacturing and refurbishing of components as these weapons age. Using conventional machining techniques to remanufacture or refurbish the special nuclear materials contained in the weapons may cause undesirable contamination, and these techniques, because they are not delicate enough, could destroy an unacceptably large part of the structure, requiring its replacement.

Building on capabilities developed for laser isotope separation programs, LDRD researchers have developed advanced lasers to perform sophisticated machining activities on nuclear weapon components. The researchers developed a theoretical understanding of laser-metal interactions at superhigh irradiances; developed numerical models based on this understanding; validated their models by comparisons with experiments; and are now using this understanding to optimize performance of the lasers in particular applications such as machining of nuclear weapon components.

LDRD researchers have developed a petawatt laser (1,000 joules in 1 picosecond), whose initial purpose was to explore a potentially more-efficient and less-expensive mechanism for laser fusion. Construction of the petawatt laser required the development of many new technologies, one of which is directly applicable to the development of short-pulse, high-power lasers for machining applications. The basic research in short-pulse, laser-material interactions provided information, which, when used with laser-materials machining codes, indicated that very accurate and delicate material cutting was feasible.

Results from the LDRD machining investigations show that high-power, short-pulsed lasers like those first developed by LDRD researchers can cut special nuclear materials with the required fine precision, making it possible to remanufacture weapons systems in an environmentally benign and cost-effective manner. Applications of these lasers to science-based stockpile stewardship are expected to save the Nation hundreds of millions of dollars in weapons remanufacturing costs.

Directed-Light Fabrication of Weapon Components. LDRD researchers have developed a new fabrication process called directed-light fabrication (DLF), and they are exploring its application to nuclear weapons fabrication (beryllium, uranium, and plutonium components). The DLF process is an automated, rapid, one-step method of making complex metal parts by fusing metal powder in the focal zone of a laser beam. A positioning system, programmed for each part's design, moves a laser beam along the contours of the part as metal powder is fed into the beam spot and fused, one layer at a time. The resulting parts are fully dense, have excellent structural properties, and are shaped to within a few thousandths of an inch of final tolerance without the use of a mold, pattern, or forming die. The system is highly flexible; operators can change to new shapes by downloading a new computer file into the positioning system. The high-energy density of the laser permits fusing of any metals, including refractory metals that are hard to form with conventional techniques. The process is ideal for low-volume production of precision parts for both defense and civilian applications. The LDRD-developed DLF process won a 1994 R&D 100 Award.

Casting Technologies. FastCast is a process for integrating computational simulation, rapid prototyping, and casting technologies into an architecture that enables the designer to go from "art-to-part," bypassing traditional machining operations. Seed funding provided by the LDRD program provided the underlying technology for the FastCast process. Before FastCast, it took 50 to 70 weeks to manufacture the first stockpile-quality fireset housing. As a result of the long delivery times, designers almost always produced the first article and subsequent development units on a milling machine. Thus, an expensive process was locked into the production stream, and, in many cases, months were required for delivery of the first item. The FastCast technology has made possible the delivery of fireset housings within ten working days of receipt of the electronic design. A consortium called FastCast, Inc., consisting of 15 companies, has been formed to support and guide this technological development.

Baseline casting technology for fabricating plutonium parts in the Pit Rebuild Program uses shaped, reusable metal molds heated above the melting point of plutonium. This technology does not address the effects of high thermal gradients, phase transformation, or development of residual stress during solidification; nor does it address distortion of the plutonium part after solidification, cooling, and final heat treatment. LDRD researchers are investigating a new approach for improving overall product quality and decreasing process complexity while simultaneously reducing the waste stream and worker exposure. The study involves developing improved casting processes using ambient-temperature molds and numerical tools to predict phase transformation, thermal behavior, residual stresses, and distortion during plutonium casting. If proven practical, the ambient-temperature mold concept will simplify casting-furnace design and reduce the heat-treating time necessary to produce the required homogeneity in the plutonium part. LDRD researchers are also developing computer simulation programs to predict distortion, residual stress, and thermal management in cast plutonium parts. Advances in these areas will benefit both the Advanced Design and Production Technology (ADaPT) and Accelerated Strategic Computer Initiative (ASCI) activities of the DOE.

Extreme Ultraviolet Lithography. The DoD and DOE defense programs rely heavily on microelectronics to provide qualitative superiority over potential adversaries. Advanced communication using miniaturized, low-power phones; ultraprecise navigation with portable global-positioning satellite equipment; and fast, on-board signal processing are but a few examples. Advanced lithography, or pattern transfer, is the key driver for all microelectronics. Industry expects a 70 percent reduction in the size of microelectronics every three years. Until now, lithography has been able to meet this demand by using ever-decreasing exposure wavelengths down into the ultraviolet region of the spectrum. However, the present lithographic approaches cannot be extended further because of material limitations. There are no lens materials that are transmissive below 180 nanometers. New approaches must be developed and commercialized to meet the industry needs.

As early as 1989, work on a new approach using extreme ultraviolet (EUV) wavelengths and reflective mirrors to achieve 0.1-micron resolution was made possible by LDRD work on EUV source technology. The success of this LDRD-supported research led to a major technology transfer initiative (TTI) program that resulted in several cooperative research and development agreements that are coordinated by a DOE-appointed Industrial Advisory Board. The TTI program has resulted in several significant advancements, including the only fully integrated 0.1-micron EUV lithography tool in the world, which has put the United States at least two years ahead of both Japanese and European efforts and allowed fabrication of the world's smallest device using projection lithography. This work required state-of-the-art advancements in wafer stages, resists, sources, cameras, and control systems. The EUV lithography tool is now being used to fabricate miniaturized sensors with unprecedented sensitivity and novel microstructures for applications in materials management and nonproliferation. Recently, it has been used to fabricate the world's smallest digital hologram for possible defense applications.

Robotics for Advanced Manufacturing and Dismantlement. The Intelligent Systems and Robotics Center (ISRC) was created almost ten years ago to provide R&D support of DOE needs in defense programs and environmental remediation. LDRD funding has played a central role in developing the ISRC's current capabilities and making it the leading robotics R&D center in the United States. The ISRC's activities span the gamut from research through development to application, with LDRD providing key funding at the "head of the pipeline." Fielded systems for weapons dismantlement, pit storage and monitoring, and deployment of systems for component manufacture have relied heavily on LDRD-funded developments in robot control, force sensing, and system software.

Several current LDRD activities are on a fast track to affecting advanced manufacturing operations in weapons production. One of these, the Archimedes assembly planning system, can read the designer's computer-aided-design files and create feasible assembly sequences that influence the manufacturability of a product and, consequently, provide important feedback to the designer. In addition, scientists are exploring the use of Archimedes in the development of training videos to allow field modifications of existing weapons. Another LDRD activity is exploring applications of the HoldFast fixture design system to the production of neutron generators. Fixturing is an important roadblock and major expense in this and similar production activities. The HoldFast approach appears to have a high likelihood of reducing both the time and cost of acquiring fixtures. These advanced manufacturing technologies, which were developed by LDRD researchers, are leading to reduced costs, improved response, and better product performance in the manufacture of weapons components.

Other Special Nuclear Materials (SNM) Manufacturing Technologies. In addition to the radioactive and biochemical dangers that special nuclear materials possess, they have many unusual physical properties that make their fabrication difficult. It became clear that it was important to study the possibility of using advanced fabrication techniques for new nuclear weapons production facilities. The objective was to develop more compact and efficient manufacturing processes with environmentally less burdensome waste streams and a more healthful environment for workers.

LDRD activities to support this objective have centered around three major activities: special materials waste streams, net-shape materials forming, and radiation dosimetry. Activities relating to materials waste streams have been very successful, and their results are already incorporated into most of the new plant concepts. In net-shape forming, recent LDRD work involves both the finite-element analysis of uranium spin-forming and the alloying chemistry of uranium. In the latter case, the research seeks to create uranium alloys that have the desired weapons-physics properties and that meet future weapons-complex fabrication requirements. In the former case, the research seeks to determine the control parameters for spin-forming uranium parts by using the extensively developed, elastic-plastic, finite-element mechanics codes (e.g., Nike and Topaz) together with constitutive-equation measurements. This problem is important because spin-forming is a natural net-shape production process for the nuclear weapons program. A forming machine has been procured; a controller is being refitted with new sensors and algorithms that use the results of the LDRD research; and state-of-the-art spin-forming will be undertaken during the coming year. In radiation dosimetry, a very important experiment funded by LDRD has indicated that exposure to radiation is somewhat less dangerous than previously thought and that the present DOE standards are safe and can be used for future stockpile activities.

Advanced Computational Capability and Nuclear Weapons Simulation

Computer simulation of the complex phenomena that occur in a nuclear explosion continues to tax available computational capabilities and simulation techniques. LDRD funds have been invested over the years in exploratory aspects of advanced computing and have been instrumental in advancing the computational capability at the three nuclear weapons laboratories. The ability to predict with confidence the performance of nuclear weapons based on computer simulations without reliance on nuclear testing is key to maintaining a safe, secure, and reliable stockpile for the foreseeable future.

Massively Parallel Computers. LDRD researchers have made significant contributions to the development of both hardware and software for high-performance computing at the nuclear weapons national laboratories. For example, during the last decade, it became apparent that mass-produced computer-processor chips, if assembled together into a massively parallel computer, could produce a thousand-fold increase in our capacity to simulate complex physical conditions; this capacity increase was necessary for our national security missions. The most pressing unanswered questions were (1) How does one wire these “commodity chips” together? and (2) How does one write the software? The three weapons laboratories began their exploration of these questions by acquiring several different types of computing machines made from these chips, exploring the writing of the types of software needed for national security problems, and investigating the closely related problems of memory sizes, networks, display techniques, and operating systems.

LDRD researchers investigated a series of experimental computers, including the multiple-instruction multiple-data architecture, with coherent and distributed memories. These researchers found that limitations in data storage and network architectures were bottlenecks in solving national security problems and that these bottlenecks were not being adequately addressed by the commercial community. LDRD funds were used to initiate a joint Computer Storage Project (CSP) between the laboratories and the commercial sector. The CSP is resolving these “bottleneck” problems and is providing enabling technology to commercial suppliers.

Another LDRD effort in high-performance computing brought together a team made up of computer system designers and computer system users who were tackling very complex problems such as nuclear weapons design and global climate modeling. The team investigated possible computer architectures and systems and applications software that could address complex problems that simultaneously require both the ability to handle huge ranges in the time and space scales and the ability to simulate the immense complexity of the many interacting phenomena in such problems. This LDRD work has provided enabling technology for the development of the “Connection Generation” of computational machines that employ massively parallel architecture. Connection Machines are now regularly used as part of the nuclear weapons program computational base, where much larger computational needs are driven by the cessation of underground nuclear testing.

Data-Transfer Network and Multimedia Technology. Computer simulation of nuclear weapons requires not only the most powerful computers available but also the ability to transfer huge amounts of computational data and the capability to display this data in forms that can be more easily understood and analyzed. LDRD researchers have pushed fast, data-transfer network technology, making it now possible to use the combined computational power of supercomputers at several locations (e.g., at the three nuclear weapons laboratories) to solve very large, complex problems.

This research resulted in the invention of the high-performance parallel interface (HIPPI), which supports local networks at data-transfer rates of 800 million bits per second and has been adopted as a standard by the American National Standards Institute. HIPPI has been implemented in many vendors' equipment and is currently the high-speed interface of choice in the supercomputer arena. Built on the LDRD work, a gateway has been developed that can link supercomputers at HIPPI speeds over very large distances. The gateway creates networks that can send the equivalent of one-hundred, 250-page books across the country in one second. This invention received an R&D 100 Award in 1995.

Asynchronous transfer mode (ATM) technology is the basis upon which Defense Programs’ (DP’s) high-performance Accelerated Strategic Computing Initiative (ASCI) network is being designed. LDRD has contributed to the understanding of traffic-management issues in high-speed ATM networks. In particular, a Monte Carlo (MC) simulator was written to model the various components in an ATM network and was used to study data-transfer congestion. It was shown that performance is very sensitive to data loss in ATM networks; that is, a small percentage of data loss results in a high level of degradation in the performance of an application. As ATM technology is being deployed to alleviate bandwidth bottlenecks, congestion issues become increasingly important. This LDRD work is providing the understanding and insight that can lead to better network switch design, to improved network resource provisioning, and to effective network management.

Modern engineering requires increased collaboration and communication between designers, analysts, and manufacturers who are located in separate facilities and even in separate states. More and more, these sources of information are producing multimedia results: video and still images of test results, plots of sensor data, electronic drawings of parts, and annotations of processes by text or audio. This type of environment requires diverse sets of applications, including sharing, archiving, retrieving, broadcasting or multicasting, searching, and linking of multimedia data streams. The distributed audio/video environment (DAVE) is a model that integrates multimedia-ready computers into a distributed multimedia environment. The initial funding for DAVE came from an LDRD activity to develop a heterogeneous video-conferencing environment that includes multiparty video conferencing and application sharing. DAVE is widely used and is the premier method for transporting high-speed, high-bandwidth, high-frame-rate, real-time video over computer networks.

Nuclear Weapons Simulation Methods. LDRD researchers have been instrumental in developing the tools needed to model radiation (neutrons and photons) and material flows in nuclear devices. LDRD work led to the development of the discrete ordinates (Sn) method for radiation transport, the particle-in-cell method for hydrodynamics, and other computational tools that are used widely today. Current LDRD research in this area is providing the technology to implement these tools on the new generation of massively parallel supercomputers. For example, a current LDRD project is providing important new capabilities that include a complex geometric representation common to both MC and Sn codes; an automatic, three-dimensional MC variance-reduction algorithm; and massively parallel, high-order-accurate, deterministic transport methods capable of modeling complex, three-dimensional geometries. Another LDRD activity is restructuring a prototype three-dimensional hydrodynamics code on the T3D computer; implementing and evaluating adaptive mesh refinement techniques; and developing innovative algorithms involving volume/interface tracking, advection, and interfacial flow for improved simulation fidelity and efficiency.

Engineers design and simulate the performance of new products, whether automobiles or nuclear weapons, by first creating a spatial-mesh model of the object. This mesh-generation task has traditionally been a highly challenging and time-consuming portion of the overall analysis. As computational capability increases, the size and scope of analyses performed have increased proportionally, further complicating the mesh-generation task and creating a bottleneck in the simulation process. LDRD researchers are investigating approaches to solving this problem. One outcome of this research is a new patented algorithm called "paving," which fills an arbitrary, three-dimensional surface with quadrilateral elements. This all-quadrilateral mesh can be made both very efficient and accurate, making it very desirable for analysis. Because the process is automated even for very irregular shapes, it saves the analyst time that can be used for more in-depth and exhaustive analysis and testing. For complicated cases, the algorithm may produce a mesh three to ten times faster than current manual methods. Paving can also be used to modify and improve a mesh during analysis, a process called adaptivity, which can take the guesswork and error out of constructing a finite-element mesh. The paving algorithm has had immediate impact on the user community, and hundreds of analysts are using it to increase their productivity.

Neutron-Scattering Science and Accelerator Technology for Stockpile Stewardship

LDRD investments in neutron-scattering science are making significant contributions to stockpile stewardship by providing advanced capabilities for examining the condition of nuclear device components. In addition, LDRD has provided the initial impetus for several accelerator-driven transmutation technologies (ADTTs), including accelerator production of tritium (now a major DOE programmatic effort).

Neutron-Scattering Diagnostic Capabilities. During the past few years, LDRD investments in neutron-scattering science diagnostics at the Manuel Lujan Neutron Scattering Center (MLNSC) have provided new capabilities that are enhancing the ability to carry out the stewardship mission in a nontesting environment. Specifically, LDRD investments allow neutron examination of components of a nuclear device to assess its condition through detection and measurement of changes associated with aging. An example is a small-angle scattering spectrometer that allows detection of internal cracks and voids in materials such as shaped high-explosive charges. Those small defects could cause ignition hot spots, potentially greatly reducing yield or even causing failure of a nuclear device. This instrument can also detect the presence of helium bubbles in plutonium (from alpha decay) that may induce small changes in the plutonium properties, again contributing to poor weapon performance.

Another example is development of neutron probes that can measure residual stress in engineering materials. Such stresses can cause changes in mechanical properties that have serious impact on reliability and safety. In the absence of mass production of weapon components and the resulting lack of statistical process control, such neutron probes provide the only technique for ensuring that a remanufactured component does not contain damaging residual strains.

On the analysis capability side, LDRD researchers have modified a computer code, which was designed to analyze neutron and x-ray data, to allow determination of the internal "texture" of materials. This modified code is regarded as a significant breakthrough that now allows examination of possible changes inside metallic components.

Accelerator-Driven Transmutation Technologies. Since the early 1990s, LDRD researchers have investigated and developed accelerator-based technologies such as the production of tritium, the conversion/destruction of weapons-grade plutonium, and the transmutation of nuclear waste with concurrent energy production. ADTTs use high-energy (approximately 1 gigaelectronvolt) proton beams such as those available at MLNSC to produce spallation neutrons in a target assembly. The energy spectrum of the spallation neutrons is modified using a neutron moderator, and the neutrons are absorbed and multiplied in a power-producing subcritical assembly. To produce or destroy the targeted materials, excess neutrons are either absorbed in the same assembly or in a blanket assembly. The thermal energy generated in this process is recovered to produce electrical power, which drives the accelerator (any excess electrical power goes to the electric power grid).

LDRD researchers have investigated technologies for the components involved in the various ADTT applications. As a result of this early LDRD work, accelerator production of tritium has been selected as an alternative to the traditional use of high-power, critical, nuclear reactors. If the accelerator approach is selected as the technology of choice for maintaining the nation's supply of tritium, the LDRD work will have produced a very significant contribution to stockpile stewardship and national security.

Weapon Communications

Lasers are the key to many modern electronic devices, from compact-disk players to printers to weapon communication systems. These devices currently use tiny lasers, called edge-emitting semiconductor lasers, that are grown in semiconductor chips. LDRD-funded engineers have been working to develop a vertical cavity surface-emitting laser (VCSEL) that will replace and greatly improve existing laser technology. VCSELs are grown in layers just like more familiar types of semiconductor devices. Mirrored cavities in the semiconductor emit light when supplied with electric current. VCSELs, first demonstrated in Japan, have been developed and refined by LDRD researchers since 1986. As a result of this work, the United States holds the world record for VCSEL efficiency (53%) at a 1-milliwatt power level.

VCSELs offer many advantages over existing technology. They are several hundred times smaller than edge-emitting lasers, and they produce a higher-quality, more tightly packed beam of light. This new technology enables advanced packaging of multichip modules, new nuclear safety options, and internal and external weapon communication systems. Recent LDRD work has focused on developing VCSELs for multigigabit-per-second optical data communications applications and on designing, growing, fabricating, and characterizing devices that operate at up to 20 gigahertz.

Nonproliferation, Counterproliferation, and Arms Control

Examples of LDRD contributions to national security in the areas of nonproliferation, counterproliferation, and arms control are described in this section. These LDRD efforts are advancing the science and technology required to verify and monitor arms control treaties, and to help detect the clandestine production of weapons of mass destruction such as nuclear, chemical, or biological weapons.

Advanced Gamma-Ray Detectors

LDRD research in gamma-ray imaging spectrometers and nonimaging detectors has found application to the arms inspections called for by the Strategic Arms Reduction Treaty (START).

Gamma-Ray Imaging Spectrometer. In the early 1990s, LDRD funded research on new types of gamma-ray detectors, imaging gamma-ray cameras, and the computer analysis of signals from networks of detectors. Much of this work was motivated by fundamental astrophysical investigations, but it has found its most important applications in counterproliferation and treaty verification. One particularly important development is a gamma-ray imaging spectrometer (GRIS), which consists of four coaligned, independent imagers, each with its own detector and coded aperture mask. Each detector “sees” incoming gamma rays only through its own specially coded mask, which serves as the imaging optic for the gamma rays. This mask is mounted on a movable plate in front of the detector plane; moving the plate provides different levels of zoom for the gamma-ray images. Coaligned with the gamma-ray imagers is a video camera, which provides both a visual aim point and visible light images that can be overlaid with the gamma-ray image to pinpoint the location of the radioactive material.

GRIS has found many applications, including environmental cleanup, astronomy, medicine, and nuclear power. However, its most significant application has been in arms inspections called for by the START—specifically, it has been used to count the number of warheads on board a missile without requiring either close access to the missile or its disassembly. Related applications that take advantage of GRIS’s ability to “see” behind shielding occur in nuclear waste disposal and in the characterization and safeguarding of nuclear weapons.

Nonimaging Detectors. Another LDRD-funded development, nonimaging detectors, is also finding application in counterproliferation activities. At a demonstration at a military base in Europe, these detectors were able to track the movement of a "clandestine" nuclear weapon by using a sophisticated tracking algorithm to identify the weapon's signal in a high-background environment. Eventually, this approach could be used in civilian areas such as seaports, airports, and other high-risk constricted areas.

Monitoring Devices for Nonproliferation and Arms Control

LDRD has supported the development of technologies for monitoring clandestine, as well as announced, nuclear explosions. One example, a reliable technique for on-site verification and measurement of nuclear weapon yields, has made a major contribution to the Threshold Test Ban Treaty (TTBT). The technique, continuous reflectivity radius-versus-time experiment, is based on early LDRD research into shock wave propagation. That work demonstrated geological applicability of the method and played a major role in establishing a trusted and simple measurement technique that enabled the successful and prompt conclusion of a TTBT.

The ability to detect small, clandestine, underground nuclear tests globally has become increasingly important. Another LDRD project successfully developed a new method that measures the scattered energy contained in the trailing seismic waves of an event. The key advantage of the method is that it uses seismic data from a single monitoring station, with savings in cost and ease of deployment. Another important advantage is that it can reliably distinguish small nuclear explosions from small earthquakes. The method was successfully used to analyze and discriminate data from 27 Nevada Test Site explosions and 15 southern Great Basin earthquakes of magnitudes between 3.1 and 4.7.

Earth-orbiting satellites have detected transionospheric pulse pairs that are similar to signatures generated by a nuclear explosion. LDRD scientists have developed a theoretical model that explains how these signals are produced by a runaway electron mechanism near thunderstorms that causes upward-propagating discharges called “sprites.” The theoretical predictions have been found to agree with measurements of radiofrequency “chirp” pairs, as well as with optical and x-ray emissions associated with this phenomenon. As a result of this work, scientists can now more accurately identify signals from clandestine nuclear explosions.

LDRD researchers are also developing another method to detect clandestine nuclear explosions in the upper atmosphere. This method is based on the detection of low-frequency (subaudible) sound waves, which can travel and be detected at great distances. These subaudible sound waves are rare in nature, but are generated in aboveground nuclear explosions and can be detected worldwide by a properly designed monitoring system. LDRD researchers have used subaudible sound waves generated by space shuttle launches to test and refine detection equipment, determine how to deploy it, and optimize ways to analyze the data.

Remote Detection of Chemical Plumes

The production of SNM, chemical weapons, and biological agents requires the use of certain solvents and reagents that are often released in small quantities into the atmosphere. It is possible, in principle, to detect these chemicals by using sophisticated spectroscopic techniques and laser-radar probing systems. Many challenges are associated with such detection techniques, including the influence of the atmosphere on the spectral signatures of the chemicals being detected; the optical behavior of the atmosphere and how it distorts the spatial-volume sampling profiles of the laser-probe beam; and the physics of reflection that determines the return scattering intensities.

The LDRD programs at the three nuclear weapons national laboratories have invested in a wide variety of technologies to address the challenges posed by the need to sample signature chemicals at a distance. For example, LDRD researchers have developed laser-diode arrays and new, solid-state laser materials for the production of very powerful, yet compact and efficient, laser transmitters. Other LDRD researchers have investigated the spectroscopy of known chemical reagents in the atmosphere and the propagation of laser beams and their reflections from aerosol-scattering systems and ground-based reflecting objects. The results of these LDRD studies have been incorporated into DOE’s Chemical Analysis by Laser Interrogation of Proliferation Effluents program, which is supporting development and testing of field-equipment systems capable of detecting the presence of operations in which weapons of mass destruction are being manufactured.

Satellite Remote-Sensing Science

The science and technology of satellite remote sensing is an emerging, rapidly growing, interdisciplinary field with many global and regional applications that require quantitative sensing, from space, of Earth’s surface features as well as its atmosphere. It is possible today to resolve structures on Earth's surface that are as small as one meter. If this high spatial resolution is coupled with high spectral resolution per pixel (as is possible, for example, with a spectrometer in space), instant object identification can also be achieved. To interpret these spectral signatures (e.g., for plutonium or uranium) correctly, it is necessary to perform a computational correction on the satellite imagery that removes the distorting effects of the atmosphere.

LDRD has funded research in satellite remote sensing since 1993—and much earlier for ground-based sensing using laser imaging, detection, and ranging (LIDAR). One such project focused on developing the technical basis for (1) LIDAR field measurements of wind to improve prediction of chemical and biological agent transport on the battlefield and (2) LIDAR field measurements of wind, temperature, and water vapor to improve the placement and interpretation of sampling detectors used for proliferation detection. Measurement requirements, operational platforms, and LIDAR technologies for the proliferation-detection problem have been studied, and preliminary choices for further development have been made.

A major LDRD activity in remote sensing science is underway to support expanding competencies in nonproliferation, environmental monitoring, and nuclear-waste processing. This activity is

- investigating passive remote sensing using the optical and infrared portions of the electromagnetic spectrum at high spectral resolution (hyperspectral sensing) to allow detection and measurement of "targets" that were previously washed out;
- developing the science and technology allowing lasers to be used for the active, remote sensing of atmospheric transport parameters such as winds, temperatures, and moisture content that are of great practical importance in proliferation detection; and
- developing new, remote sensing concepts—such as a practical concept for retrieving signatures of vegetation canopies that would allow identification of species and recognition of thermal or chemical stress in plants.

Forensic Science and Counterproliferation

LDRD has funded research to determine how best to measure trace materials for nonproliferation, counterproliferation, and other purposes such as forensic science. Using sophisticated analytical equipment, LDRD researchers in organic, inorganic, and biological chemistry invented and demonstrated new ways to determine the composition and, often, the sources of the most minute samples of unusual materials. The successes of these studies, which relied upon interdisciplinary approaches and risk taking with unusual techniques, led to the establishment of the Forensic Science Center in 1991. In a very short period, the Center has become a leader in law enforcement, national security, defense, and intelligence applications. Technologies made possible by the initial LDRD funding are being used to verify and monitor compliance with such international agreements as the Nuclear Nonproliferation Treaty and the Chemical Weapons Convention and are also being used to learn whether a country is developing a clandestine nuclear weapons program.

LDRD has supported other innovative developments such as combining three technologies into a single system; these three technologies are an ion-trap mass spectrometer for analysis, a high-powered microscope for viewing, and a laser for ionizing samples. In this system, sampling material is placed on the tip of a probe that is inserted into the source region of an ion-trap mass spectrometer. With a microscope outside the vacuum chamber, the sampling material is viewed from above at a magnification of 250 times. A laser beam is then directed at precisely the 10- to 50-micrometer spot on the probe tip from which the sample's mass spectral data are desired. The intensity of the laser beam can be adjusted to vaporize instantaneously either more or less sampling material, depending on the size of the sample. The laser ionizes the material, and the mass spectrometer sorts these fragments according to their molecular weights. Once sorted, each chemical component produces a characteristic mass spectral fragmentation pattern that is used by the operator to identify the entire sample. Although this technique is still in its infancy, its potential could be enormous in forensic investigations related to nonproliferation and counterproliferation as smaller and smaller particles and fibers can be sampled and characterized.

LDRD also has funded the development of a suitcase-sized gas chromatograph/mass spectrometer for on-site identification of ultratrace (microgram or less) quantities of certain compounds in complex mixtures.

The system weighs 20 kilograms, including an accompanying laptop computer, can be carried onboard an airplane, and can be placed into the overhead compartment. Meanwhile, its accompanying generator and off-line vacuum-reconditioning pumping unit travel in the baggage compartment. This system is finding application in nonproliferation activities.

Global Nuclear Material Flow Model

The global proliferation of weapons-grade plutonium and highly enriched uranium has become one of the foremost threats to global security. This nuclear danger can be reduced by a system for global management, control, and disposition of special nuclear materials to prevent their use for weapons purposes. LDRD researchers are characterizing and modeling, from a global perspective, the management, control, and flow of weapons-grade nuclear materials. The objective of this work is to provide a computer-based tool capable of

- capturing and enumerating the information and data concerning the global inventory of nuclear weapons materials;
- providing a global view of the management and control of nuclear materials, including resource and accounting requirements;
- undertaking macrosystem simulations of safeguards-accounting surety and safeguards-resource estimation for the management and control of nuclear materials;
- visually representing the information related to nuclear materials (e.g., management and control, quantity, location, and transit) and both the intercountry and intracountry flow of nuclear materials; and
- supporting the development of other pertinent algorithmic capabilities necessary to undertake further global studies related to the management and control of nuclear materials.

Significant progress has been made toward these objectives, including development of a prototype of the fundamental, computer-based framework necessary to undertake these studies. It is expected that this tool will help answer questions concerning the degree of certainty associated with estimating material quantities based on inventory information, safeguards-accounting information, and material transit. It should also provide the framework, initial data, and information necessary for conducting optimization studies to estimate safeguards-resource requirements based on the existing safeguards resources, management and control requirements, and changing assurance needs.

Nuclear Materials and Defense Waste Disposal

LDRD researchers at the nuclear weapons national laboratories have contributed to a wide variety of scientific and technological areas that have led to a better understanding of plutonium and other actinide materials, as well as to advanced methods for assaying, separating, and disposing of defense wastes. Some of these contributions are detailed below.

Plutonium Equation of State

LDRD-funded researchers developed the diamond anvil cell (DAC), a versatile experimental tool for studying the properties of materials at very high pressures (>300 GPa or 3 x 10^6 atm). The DAC apparatus is well suited for investigating hazardous toxic materials because the samples required are very small (milligrams) and are easily contained. Thus, it is an excellent tool for studying the melting of toxic metals at very high pressures. More recently, a laser-heated DAC was developed by LDRD researchers who undertook a high-risk study to determine to what extent this new approach could be used for high-temperature, high-pressure SNM studies. Diamond is transparent to electromagnetic radiation and has high thermal conductivity—features that were exploited to develop the laser-heating technique in the DAC. The laser-heated DAC is placed in an x-ray beam to determine simultaneously the density and temperature of a sample at ultrahigh pressures. This allows the determination of the equations of state and the melting properties of metals and other materials in regimes that previously could only be reached during chemical or nuclear-explosion-driven experiments.

The melting curve of plutonium, one example of a measurement obtained with the laser-heated DAC apparatus, has proved to be of great interest in nuclear design because the subtle interplay of material strength and its loss caused by melting solves a long-standing problem in accurately modeling implosion devices. Precise measurements of the melting curve by LDRD scientists have enabled more accurate simulation of the distribution of solids and liquids in an imploding device. The distribution of material phases controls the initial conditions for hydrodynamic instabilities and, therefore, controls device performance. The plutonium melting curve placed constraints on calculations, leading to improved understanding of the implosion process.

Plutonium Recovery

Scientists have developed a novel one-step method for recovering metallic plutonium from nuclear weapons, a development that received a 1995 R&D 100 Award. The new method, called the hydride-dehydride recycle process, eliminates the environmental hazards associated with other plutonium recovery methods. It takes advantage of plutonium's strong affinity for hydrogen gas, a reaction that forms plutonium hydride. The reaction takes place in a vacuum chamber inside a glove box. The lower part of the chamber includes a heated crucible, and the upper part (cold zone) contains the weapon component. A small amount of hydrogen gas is introduced into the cold zone, where it reacts with the plutonium to form plutonium hydride powder. The powder falls into the hot crucible below, where the hydrogen is released (the dehydriding reaction). The hydrogen then recycles through the process until all the plutonium has been extracted from the weapon component. When the process is complete, the plutonium powder that has collected at the bottom of the crucible is melted and incorporated into a storage-ready ingot. LDRD is funding a series of laboratory-scale experiments to obtain data for enhancing the operational and safety characteristics of the hydride-dehydride recycling process for plutonium recovery. This LDRD work helps provide core technology for the DOE Advanced Recovery and Integrated Extraction System.

In a related LDRD-developed process, plutonium metal is converted to plutonium hydride and then chlorinated to form plutonium chloride and volatile chloride impurities. This technology, like the one described in the preceding paragraph, can be used to reprocess plutonium from retired nuclear weapons for use in recycled weapons, or it can provide weapons plutonium as purified feed material for mixed-oxide fuel to be burned in nuclear power reactors as part of an overall nonproliferation approach. This LDRD work has resulted in a successful feasibility demonstration that has strengthened the technology base for plutonium processing. The new technology is being considered for implementation by the DOE Fissile Materials Disposition Program.

Characterization of Actinide Materials

Understanding the chemistry and metallurgy of the actinide elements has taken on new significance in the areas of stockpile stewardship and management. LDRD researchers are contributing to this understanding by developing new neutron diffraction techniques, by investigating the crystal structures of several actinide alloys, and by developing multidisciplinary approaches to predicting the chemical and physical properties of actinide materials.

Neutron Diffraction Studies. With the end of the Cold War and the concomitant cessation of both underground nuclear testing and the manufacture of new nuclear weapons, new issues vital to the national security mission have arisen. Specific examples are long-term storage of nuclear materials and aging of plutonium in primaries in the nuclear stockpile. An LDRD activity is focusing on answering questions of practical importance to stockpile integrity and long-term storage of nuclear material. Specific areas under investigation are neutron diffraction techniques for smaller actinide samples, modeling of inelastic scattering data for actinide metal hydrides, actinide oxide structures, and aging effects in actinides. These studies use neutron scattering supported by resistivity, magnetic susceptibility, Sieverts equilibrium studies and kinetics, and x-ray diffraction. LDRD researchers have developed an encapsulation cell for small actinide samples to enable neutron diffraction studies of rare or radiologically difficult actinides. The researchers also have performed model calculations of helium ingrowth in aged plutonium at room temperature that predict bubble formation only at grain boundaries.

Actinide Crystal Chemistry. Complexity of crystal structure is the outstanding scientific problem in actinide crystal chemistry. It is not known why the idiosyncratic structures of plutonium metal occur or how they transform among themselves. The electronic instability of the 5f electronic shell that is just beginning to be filled in the light actinides causes the formation of "self-intermetallic" compounds in both plutonium metal and its alloys, and the formation of these compounds is responsible for the observed complexity of structure and phase behavior. Knowledge of the structures of elemental plutonium has not by itself led to the reliable prediction of behavior with respect to structural transitions, stability, and thermodynamic properties. An understanding that would provide real predictive power is now a requirement of the stockpile stewardship mission. Current LDRD work is contributing to this understanding by determining the crystal structures of several actinide alloys, including neptunium-uranium, plutonium-thorium, and plutonium-zirconium.

Actinide Molecular Science. The chemistry and physics of the actinide elements have always been of prime importance because they provide the basis for process and separation chemistry and metallurgy related to the nuclear weapons mission. Recently, interest in the chemistry of the actinides has taken on new significance in the areas of environmental remediation and stockpile management. However, our ability to extend our understanding of the behavior of these complex elements has been eroded by time and by the reduced flexibility of programs to address research outside of solving short-term problems. LDRD investigators are combining synthetic chemistry, spectroscopic characterization, and theory and modeling to understand and predict the chemical and physical properties of actinide materials. This multidisciplinary approach is providing the scientific means to formulate rational approaches for solving complex actinide problems in a wide variety of environments.

Long-lived actinides constitute the dominant radiological hazard to the environment associated with the nuclear fuel cycle. LDRD researchers have developed techniques to measure chemical properties of actinide element solution species, enabling follow-on work to assemble the thermodynamics database necessary to understand and model the chemical behavior of actinides in geologic repository conditions. Ultimately, this work has provided the basis for new pyrochemical processing techniques that result in far less waste than the standard aqueous treatments. The approach developed is now being applied in a prototypical production system for the DOE Fissile Materials Disposition Program. The techniques also are under consideration by the DOE Environmental Restoration and Waste Management Program for treatment of the chemically unstable residues located at many DOE sites.

Waste Disposal Technology

The LDRD programs at the three nuclear weapons national laboratories have funded research efforts designed to help understand and develop new approaches for dealing with the disposition of radioactive and other hazardous wastes that are the legacy of 50 years of nuclear weapons production. In addition to the plutonium recovery work described previously, we discuss below contributions to separations science and technology using polymers; integrated approaches for disposing of mixed (hazardous organics and radioactive) wastes; methods for nondestructively examining waste containers; radiation-hardened robots for applications to nuclear waste cleanup; and portable instrumentation for on-site analysis of solid and liquid effluents.

Separations Science and Technology. Separations science is an interdisciplinary technology that affects almost every endeavor of DOE, DoD, and US industry. Chemical waste treatment and pollution prevention are critical needs in nuclear materials control, recovery, and purification. The high cost associated with the long-term storage of radioactive wastes mandates separating the radioactive components from the nonradioactive components in a process waste stream before the waste is packaged and stored. Separation processes are also an integral part of managing the plutonium legacy. The LDRD programs at the nuclear weapons laboratories are addressing many of these issues.

For example, LDRD researchers have developed and evaluated water-soluble chelating polymers for recovery of actinide and toxic metals from a variety of process streams. The work focuses on two target areas: (1) the removal of actinides and toxic metals from wastewater, and (2) the recovery, using polymer filtration, of copper and other precious metals from industrial process streams. This LDRD work involves advanced ligand/polymer synthesis, assembly of equipment, and process demonstration. A portable polymer-filtration system based on this technology, which was used to recover zinc and nickel ions from electroplating rinse waters, won an R&D 100 Award in 1995. LDRD is now funding research in membrane-based separation technologies for the removal of plutonium and americium from nuclear materials-processing wastewater; in fission-product separations using cobalt dicarbolide for solvent extraction; in the development and application of hollow-fiber membrane modules for separating gases and nuclear materials; in selective waste remediation using *in situ* photocatalytic reactors; and in other technologies.

In another example, LDRD researchers are developing integrated approaches for the disposal of defense legacy wastes containing both hazardous organics and toxic and/or radioactive metals. These mixed wastes contain metals such as lead, chromium, and actinides; a variety of solvents such as methanol, acetone, and chlorinated hydrocarbons; and cellulose materials such as rags and paper. The complexity of the mixed waste makes it difficult to identify a single technology that will adequately address all the waste treatment issues while being, at the same time, inexpensive, safe, and environmentally benign. LDRD researchers have coupled two accepted and proven waste treatment technologies—metal extraction chemistry and biological degradation of organics—to address this legacy waste problem. The researchers have developed a chelator system, based on water-soluble polymers, that simultaneously binds both lead and chromium and that may also have potential for plutonium extraction. In addition, the researchers have identified, cultured, and tested biological degraders for target organics and cellulose and have investigated the toxicity of the waste metals relative to these cultures.

Nondestructive Assay of Nuclear Wastes. A trailer-mounted, waste inspection tomography (WIT) system, which can look into drums without opening them, uses techniques developed by LDRD researchers. These techniques, which are similar to medical x-rays and computerized axial tomography scans, are used to examine the contents of drums, including the amounts, location, and types of both radioactive and nonradioactive waste in the drums, as well as the kinds and levels of radioactivity.

Hundreds of thousands of drums of radioactive waste reside in temporary holding sites across the country awaiting the opening of permanent storage sites. Before the drums can be permanently stored, they must be inspected. The drums contain various categories of waste including low-level radioactive waste and transuranic waste (e.g., contaminated laboratory clothing, equipment, and paper towels); mixed waste (similar to the foregoing waste except that it is also contaminated with oils, solvents, or heavy metals); and high-level waste (such as spent nuclear fuel rods and vitrified wastes).

Permanent storage of these wastes will cost from $1,000 to $10,000 per drum, depending upon the kind of waste the drum contains. Accurate drum inspections will ensure that each waste container is properly stored according to its contents. The WIT system reduces drum inspection costs from a high of more than $10,000 per drum to less than $1,000. The system is faster than opening drums and eliminates the hazards of removing drum lids. The uniqueness of the WIT system is in its ability to provide quantitative results with reasonable throughput and cost. All sites that generate radioactive wastes can benefit from a safer, cheaper, and faster way to inspect waste drums.

Radiation-Hardened Robots. This LDRD effort focuses on the process of designing radiation-hardened robots for applications such as nuclear waste cleanup, nuclear plant maintenance, decontamination and decommissioning, and emergency response. The LDRD work contributes to three areas: predicting radiation doses, hardening to radiation, and monitoring doses during operation.

Predicting radiation doses uses both *a priori* knowledge of the environment, including radiation source and type, and graphical programming capabilities that are part of the robot control system. An operator can rapidly build a model of the area for application, designate objects as sources, define the source type, designate points on the robot for dose measurement, and preprogram the robot to execute a task. During simulated execution, doses accumulated at the dosimeters are tracked continuously by DoseServer, a computer code (developed by this LDRD effort) that compares the vectors from each source to each dosimeter with dose maps generated off-line. If limits designated by the operator are exceeded, DoseServer warns the operator that failure is imminent.

Hardened robotic systems can be designed using data on predicted radiation type and dose. LDRD researchers have compiled information on radiation hardness of components from weapons and space programs as well as information obtained from radiation testing of sensors and control components common to mobile, gantry, and pedestal-type robotic systems. During execution of robotic tasks in the radiation environment, a graphical user interface (part of the robot control system) tracks incoming data from radiation sensors on the robotic equipment, flagging the operator if the doses or dose rates exceed set points. This warning assists in preventing failure caused by radiation exposure by providing the opportunity to withdraw to a safer environment for preventive maintenance.

Portable Gamma- and X-Ray Detector. A new, field-portable, x-ray fluorescence (XRF) analyzer, based on large-area mercuric iodide (HgI_2) radiation sensors, has been developed by LDRD researchers for on-site analysis of solid and liquid effluents. The unit consists of a hand-held probe, which contains the HgI_2 sensor and three radioactive sources, and an XRF analyzer module, which contains a computer, software, and a display. The instrument is lightweight, easy to operate, and battery powered; it also requires no maintenance for months and is capable of remote, unattended data collection. It can quickly and nonintrusively quantify contaminants ranging from sulfur to uranium. The instrument has been used to quantify the composition and trace contaminants in a variety of specimens, and it can be used to analyze residues associated with forensic investigations (e.g., samples found at crime scenes).

In addition to the x-ray fluorescence capabilities, the XRF instrument was designed to operate as a direct gamma-ray spectrometer, and it has been used to perform nondestructive assays of radioactive gamma-emitting materials such as uranium and plutonium. The high-resolution capability of the HgI_2 sensors allows the instrument to identify radioactive materials by their unique radiological signatures, and it has been used to characterize a wide variety of nuclear materials. The sensors were also found to be radiation tolerant, with a damage threshold two to three orders of magnitude higher than cryogenically cooled silicon or germanium detectors. This feature allows their use in monitoring high-level radioactive waste or in long-term monitoring of weapon pits. Beyond the capability for monitoring stored SNM, the gamma-ray spectrometer can be used to detect nuclear smuggling, to aid in SNM search scenarios, or to perform *in situ* monitoring of airborne radioactive particulates that have been collected on filters.

Other National Security Research Areas

LDRD contributions to other national security areas include research and development of materials, detectors, and computational tools for conventional military applications, as well as sensors for environmental monitoring. Some of these contributions are described below.

Materials for Military Applications

LDRD activities at the nuclear weapons national laboratories have contributed to the understanding and development of materials for military applications. Among these materials are high explosives (HE), including insensitive HE; technology for the safe and environmentally benign destruction of HE; flexible, high-temperature superconductors (HTSCs) with world-record capabilities for carrying current; multilayer materials with applications to jet engines; and materials with strong optical shielding properties.

High-Explosives Research and Development. LDRD-funded research and development has led to numerical models that are routinely used to predict the performance and response of HE, especially insensitive HE. This work also led to the development of new explosives of choice for shape charges and development of new shape-charge technology for conventional defense. In addition, the LDRD researchers developed molten-salt technology for application to the safe and environmentally benign destruction of high explosives. This technology has been transferred to the military.

High-Temperature Superconductors. HTSCs, which can carry electrical currents without resistance at relatively high temperatures, have the potential for very broad military and civilian applications and could be influential in many applied areas such as superconducting components, ferroelectric memory elements, optical wave guides and switches, chemical sensors, and infrared detectors. Longer-range applications include power-generation devices and mass transportation.

Controlling the microstructure, composition, and mechanical properties of these many-component ceramic materials has been a barrier to implementation of this new technology. LDRD researchers were the first to discover and begin to understand the growth mechanism in films of the superconductor yttrium-barium-copper oxide (YBCO). This work has uncovered the role of film-deposition parameters in determining the film-growth mechanisms and the resulting microstructures, which in turn have a profound effect on the film properties.

Using their new knowledge, the LDRD researchers recently achieved a world-record current density of over one million amperes per square centimeter for a flexible HTSC at the temperature of liquid nitrogen (77 degrees kelvin). This one-hundred-fold increase over the previous world record is a new milestone in superconductivity and is a giant step toward practical applications. Superconductivity at the relatively high temperature of liquid nitrogen is desirable because a liquid-nitrogen cooling system is relatively easy to insulate, and liquid nitrogen is plentiful and inexpensive. Also, because the tape is flexible, it can be adapted to more uses than superconductor technologies that rely on ceramic powders in tubes. Unlike HTSCs made out of other materials, the YBCO superconducting tape retains much of its current density in high magnetic fields. All these properties result in tremendous potential for both military and commercial applications.

Multilayer Materials and X-Ray Mirrors. LDRD researchers have developed very thin, well-controlled multilayer materials and aerogels that have found application in power sources, jet engines, and x-ray lithography. X-ray mirrors developed by LDRD researchers played a dramatic role in the diagnostics of nuclear weapons during the last years of testing and are crucial elements in the National Ignition Facility target-diagnostics program.

Optical Shields For Defense Applications. Glass with an admixture of buckminsterfullerene (C_{60}) has been shown to have strong, optical-shielding properties, with applications to military defense. The geometry of the C_{60} molecule looks like the seams on a soccer ball—giving rise to the name “buckyballs.” These molecules limit light transmitted through them to an intensity below some finite threshold. Once the incoming light goes above that threshold, the molecules let no more light pass.

While this effect had previously been demonstrated in a liquid solution, LDRD researchers have now successfully formed a solid matrix containing the C_{60} molecules and have demonstrated that the doped glass exhibits the same optical-limiting properties as were previously observed in the liquid. The optical shutdown is fast, which is important when protecting against intense, pulsed-light sources. The LDRD team recently showed that special, chemically modified fullerenes, which are more soluble than C_{60}, can now be used to make high-concentration glass admixtures. This means that the fast optical-shutdown effect can now be produced in thin, protective coatings and filters. These materials provide protection that matches the wavelength of the new tunable military lasers, which produce very short, high-power pulses. By enabling the development of goggles, airplane canopies, filters, or coatings to shield eyes, equipment, and sensors from high-energy laser light, the new materials can counter the threat of tactical laser weapons. The LDRD researchers have been awarded a patent for their novel process.

Detectors for Military Applications

LDRD activities at the nuclear weapons national laboratories have enabled development of a variety of detectors for military applications, including detectors that monitor cracks and other flaws in commercial and military hardware; smart fuses for military ordnance; micropulse radars for mine detection; synthetic aperture radars (SARs) for space applications; advanced target recognition systems for mobile target detection; and an ion mobility spectroscopy (IMS) tool for explosives sensing.

Ultrasound Identification of Failure in Military Hardware. Resonant ultrasound spectroscopy (RUS) was originally used by LDRD scientists as a research diagnostic to measure the properties of high-temperature superconducting crystals. It was quickly determined that RUS could be used for the nondestructive testing of crystals for imperfections in the crystal structure. The technique was further applied to monitor for cracks and other flaws in commercial and military hardware. Detectors and diagnostic electronics that could be incorporated in industrial production lines quickly yielded spectacular results when compared with other sampling techniques being used for manufacturing quality control.

RUS is being used in the military sector for the nondestructive testing of aircraft landing assemblies, turbine disks, and ball bearings; and an effort is in progress to examine helicopter rotor parts for cracks and flaws. In an application to stockpile stewardship, LDRD researchers are exploring the use of RUS to study the effects of aging on hemispherically shaped explosive charges. Specific aging effects in weapon components include flaws, chemical migration, and debonding in the explosive fabrications.

The identification and development of RUS is an excellent example of how LDRD research that was initiated to answer a scientific question can find important applications in both the military and commercial sectors. Applications of RUS built on the foundations provided by the LDRD research have earned RUS several patents and two R&D 100 Awards.

Smart Fuses and Micropulse Radar. LDRD investigations in the area of hard-wired neural nets have led to smart fuses for military ordinance. LDRD researchers have developed high-power micropulse radar and sophisticated algorithms for detecting submerged objects. This technology, besides having numerous commercial applications, is being evaluated by the military for mine detection, seeing through walls, and military medicine.

Synthetic Aperture Radar. Work on the SAR began as a result of unique expertise gained during development of nuclear radar fuses in the 1970s and 1980s, which led to an exploratory program using advanced imaging radars for possible weapon guidance in the late 1980s. This program, in turn, led directly to the development in the early 1990s of a unique airborne SAR prototype for all-weather, long-range surveillance and reconnaissance. Since that time, LDRD researchers have advanced the SAR technology by studying its application in space; developing a unique, three-dimensional interferometric SAR; and extracting target coordinates and features from SAR imagery.

Automated Target Recognition Technology. As SAR technology makes the transition to industry and as battlefield SAR systems on tactical aircraft become more common, the amount of SAR imagery that must be handled and analyzed will increase dramatically. Handling the increased amount of SAR imagery and the timely identification of time-critical targets (for example, mobile targets such as SCUD missile launchers) using SAR imagery require automated target-recognition (ATR) systems that can quickly scan the imagery and identify areas of interest for image analysis by humans. In parallel with the SAR work described above, LDRD researchers are investigating ATR systems for time-critical mobile target detection using SAR imagery. The primary focus of this work is on multiple-source data fusion, feature extraction, and neural-net exploration.

Ion Mobility Spectroscopy for Explosives Detection. LDRD-funded work is developing IMS as a tool for rapidly screening environmental sites for the presence of explosives; to confirm the presence and/or identify unknown explosive materials in forensics investigations; to determine the contents of unexploded ordnance; and to detect concealed explosives carried by people. IMS sensing of explosives has been demonstrated in both air and water, and a robotic platform is being designed for unattended sample collection and analysis.

Computational Tools for Military Applications

LDRD researchers have contributed new modeling capabilities to the CTH computer program, a software system that is used for analyzing problems involving intense, impulsive loading of materials and structures. One example is a material-response model for materials such as layered composite materials that possess a preferred orientation. This transverse isotropic (TI) model, as implemented in CTH, models the dynamic mechanical response of a number of advanced materials that are used in nuclear weapons systems. For example, the TI model can be used to represent the tape-wrapped, carbon-phenolic composite material that is used in the aeroshell of ballistic missiles. Another application is the modeling of the polar ferroelectric materials that are found in shock-actuated power supplies for some weapon components. The TI model has been developed with a significant amount of versatility in mind. Consequently, the model provides an excellent foundation upon which more sophisticated plasticity and fracture models can be built without compromising the underlying TI symmetry of the material.

LDRD researchers also developed new capabilities for modeling dynamic fragmentation events in CTH. The main accomplishment of this effort was incorporating—in the CTH code—a means for determining average fragment size in such events. This capability has been used in defense-related applications such as formation of fragments in explosive accidents involving nonnuclear detonation of warheads, destruction of conventional explosive weapons, and debris formation during high-velocity impact.

Sensors for Environmental Monitoring

The LDRD programs at the nuclear weapons national laboratories have funded fundamental and applied research on sensors for environmental monitoring of defense wastes and for detecting environmental indicators of weapons production. Some examples include the following.

Exhaust Gases and Volatile Organic Compounds. Using molecular self-assembly techniques, LDRD researchers have developed a compact and robust surface-acoustic-wave-based chemical microsensor for remote, real-time reversible sensing of volatile organic compounds. Self-assembly techniques allow toxin-sensing molecules to organize (or self-assemble) so that one end of the molecule bonds directly to a sensing detector (a transducer) and the other end extends as a ‘bucket’ tailored to temporarily trap specific chemicals. Changing the size and polarity of the bucket allows the microsensors to be custom tailored so that they track specific organic toxins. The organic sensing layer (or bucket) is designed and constructed using molecular-engineered cyclodextrin derivatives, which provide a cone-shaped molecular structure that can readily trap specific organic toxins. Because the cyclodextrin buckets bind the contaminants weakly, the microsensor is reversible and can be used to monitor continuously changing concentrations of the contaminant over an extended period of time. This LDRD-developed technology received an R&D 100 Award in 1995.

Waterborne Contaminants. LDRD researchers have developed quartz resonator sensors for monitoring waterborne contaminants. This technology has been proposed to DOE’s Office of Nuclear Nonproliferation as a means to detect chemicals that would indicate weapon production. Inspectors could use such sensors to monitor liquid effluents from plants suspected of producing chemical, nuclear, or biological weapons. Thus, these sensors can contribute to treaty verification efforts. ■

List of Acronyms

ADaPT Advanced Design and Production Technology (DOE initiative)

ADTT accelerator-driven transmutation technologies

AEDA Atomic Energy Defense Activities

AL Albuquerque Operations Office (DOE)

ANSI American National Standards Institute

ARIES Advanced Recovery Integrated Extraction System

ASCI Accelerated Strategic Computing Initiative (DOE)

ATM asynchronous transfer mode

ATR automated target recognition

CSP Computer Storage Project

DAC diamond anvil cell

DAVE distributed audio-video environment

DLF directed-light fabrication

DoD Department of Defense

DOE Department of Energy

DP Defense Programs

EUV extreme ultraviolet

GC/MS gas chromatograph/mass spectrometer

GRIS gamma-ray imaging spectrometer

HE high explosives

HIPPI high-performance parallel interface

HTSC high-temperature superconductor

IMS ion mobility spectroscopy

ISRC Intelligent Systems and Robotics Center

MLNSC Manuel Lujan Neutron Scattering Center

LDRD Laboratory Directed Research and Development

LIDAR laser imaging, detection, and ranging

MC Monte Carlo

MILSI multiple imaging of laster-sheet illumination

NSTC National Science and Technology Council

OAK Oakland Operations Office (DOE)

R&D research and development

RUS resonant ultrasound spectroscopy

S&T science and technology

SAR synthetic aperture radar

SAW surface acoustic wave

SBSS science-based stockpile stewardship

Sn discrete ordinates

SNM special nuclear material

SONET	synchronous optical network
START	Strategic Arms Reduction Treaty
TI	transverse isotropic
TTBT	Threshold Test Ban Treaty
TTI	technology transfer initiative
VCSEL	vertical cavity surface-emitting laser
WIT	waste inspection tomography
XRF	x-ray fluorescence
YBCO	yttrium-barium-copper oxide